United States
Environmental Protection
Agency

ProUCL Version 5.1
User Guide

Statistical Software for Environmental Applications for Data Sets with and without Nondetect Observations

RESEARCH AND DEVELOPMENT

EPA/600/R-07/041
October 2015
www.epa.gov

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Statistical Software for Environmental Applications for Data Sets with and without Nondetect Observations

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NOTICE

The United States Environmental Protection Agency (U.S. EPA) through its Office of Research and Development (ORD) funded and managed the research described in ProUCL Technical Guide and methods incorporated in the ProUCL software. It has been peer reviewed by the U.S. EPA and approved for publication. Mention of trade names or commercial products does not constitute endorsement or recommendation by the U.S. EPA for use.

- All versions of the ProUCL software including the current version ProUCL 5.1 have been developed by Lockheed Martin, IS&GS - CIVIL under the Science, Engineering, Response and Analytical contract with the U.S. EPA and is made available through the U.S. EPA Technical Support Center (TSC) in Atlanta, Georgia (GA).

- Use of any portion of ProUCL that does not comply with the ProUCL Technical Guide is not recommended.

- ProUCL contains embedded licensed software. Any modification of the ProUCL source code may violate the embedded licensed software agreements and is expressly forbidden.

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With respect to ProUCL distributed software and documentation, neither the U.S. EPA nor any of their employees, assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed. Furthermore, software and documentation are supplied "as-is" without guarantee or warranty, expressed or implied, including without limitation, any warranty of merchantability or fitness for a specific purpose.

ProUCL software is a statistical software package providing statistical methods described in various U.S. EPA guidance documents. ProUCL does not describe U.S. EPA policies and should not be considered to represent U.S. EPA policies.

Minimum Hardware Requirements

ProUCL 5.1 will function but will run slowly and page a lot.

- Intel Pentium 1.0 gigahertz (GHz)
- 45 MB of hard drive space
- 512 MB of memory (RAM)
- CD-ROM drive or internet connection
- Windows XP (with SP3), Vista (with SP1 or later), and Windows 7.

ProUCL 5.1 will function but some titles and some Graphical User Interfaces (GUIs) will need to be scrolled. Definition without color will be marginal.

- 800 by 600 Pixels
- Basic Color is preferred

Preferred Hardware Requirements

- 1 GHz or faster Processor.
- 1 gigabyte (GB) of memory (RAM)
- 1024 by 768 Pixels or greater color display

Software Requirements

ProUCL 5.1 has been developed in the Microsoft .NET Framework 4.0 using the C# programming language. To properly run ProUCL 5.1 software, the computer using the program must have the .NET Framework 4.0 pre-installed. The downloadable .NET Framework 4.0 files can be obtained from one of the following websites:

- http://msdn.microsoft.com/netframework/downloads/updates/default.aspx
  http://www.microsoft.com/en-us/download/details.aspx?id=17851
  Quicker site for 32 Bit Operating systems

- http://www.microsoft.com/en-us/download/details.aspx?id=24872
  Use this site if you have a 64 Bit operating system

Installation Instructions when Downloading ProUCL 5.1 from the EPA Web Site

- Download the file SETUP.EXE from the EPA Web site and save to a temporary location.

- Run the SETUP.EXE program. This will create a ProUCL directory and two folders: 1) The USER GUIDE (this document), and 2) DATA (example data sets).

- To run the program, use Windows Explorer to locate the ProUCL application file, and Double click on it, or use the RUN command from the start menu to locate the ProUCL.exe file, and run ProUCL.exe.

- To uninstall the program, use Windows Explorer to locate and delete the ProUCL folder.

Caution: If you have previous versions of the ProUCL, which were installed on your computer, you should remove or rename the directory in which earlier ProUCL versions are currently located.

Installation Instructions when Copying ProUCL 5.1 from a CD

- Create a folder named **ProUCL 5.1** on a local hard drive of the machine you wish to install ProUCL 5.1.

- Extract the zipped file **ProUCL.zip** to the folder you have just created.

- Run **ProUCL.exe**.

Note: If you have extension turned off, the program will show with the name **ProUCL** in your directory and have an Icon with the label **ProUCL**.

Creating a Shortcut for ProUCL 5.1 on Desktop

- To create a shortcut of the ProUCL program on your desktop, go to your ProUCL directory and right click on the executable program and send it to desktop. A ProUCL icon will be displayed on your desktop. This shortcut will point to the ProUCL directory consisting of all files required to execute ProUCL 5.1.

Caution: Because all files in your ProUCL directory are needed to execute the ProUCL software, one needs to generate a shortcut using the process described above. Simply dragging the ProUCL executable file from Window Explorer onto your desktop **will not work successfully** (an error message will appear) as all files needed to run the software are not available on your desktop. Your shortcut should point to the directory path with all required ProUCL files.

ProUCL 5.1

Software ProUCL version 5.1 (ProUCL 5.1), its earlier versions: ProUCL version 3.00.01, 4.00.02, 4.00.04, 4.00.05, 4.1.00, 4.1.01, and ProUCL 5.0.00, associated Facts Sheet, User Guides and Technical Guides (e.g., EPA 2010a, 2010b, 2013a, 2013b) can be downloaded from the following EPA website:

http://www.epa.gov/osp/hstl/tsc/software.htm
http://www.epa.gov/osp/hstl/tsc/softwaredocs.htm

Material for ProUCL webinars offered in March 2011, and relevant literature used in the development of various ProUCL versions can also be downloaded from the above EPA website.

Contact Information for all Versions of ProUCL

Since 1999, the ProUCL software has been developed under the direction of the Technical Support Center (TSC). As of November 2007, the direction of the TSC is transferred from Brian Schumacher to Felicia Barnett. Therefore, any comments or questions concerning all versions of ProUCL software should be addressed to:

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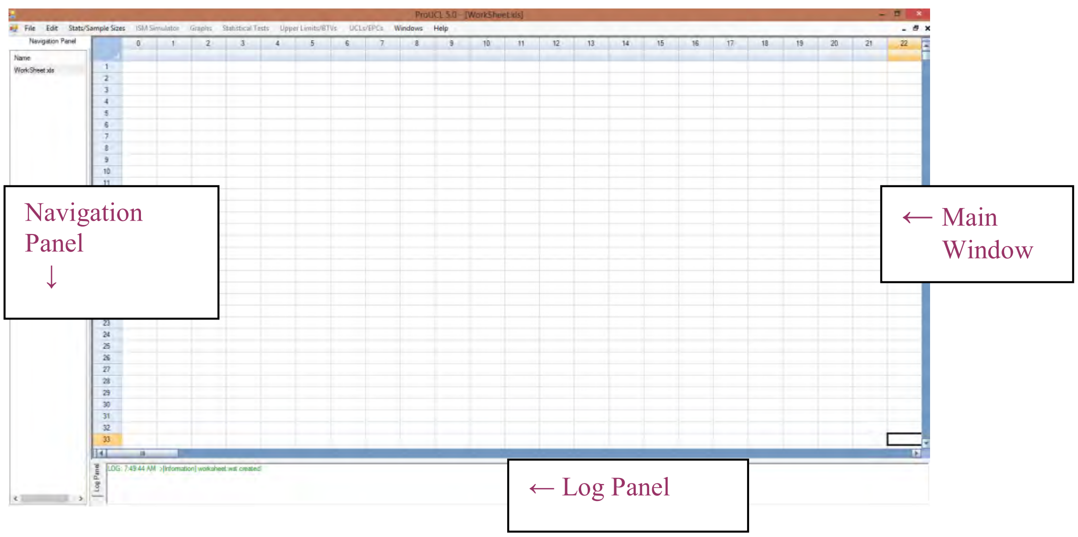
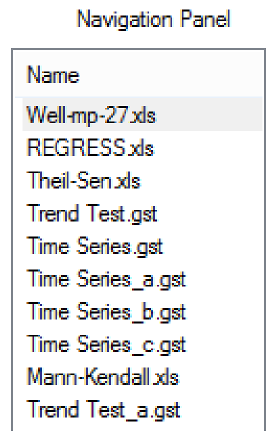
Getting Started

The look and feel of ProUCL 5.1 is similar to that of ProUCL 5.0; and they share the same names for modules and drop-down menus. The functionality and the use of the methods and options available in ProUCL 5.1 have been illustrated using Screen shots of output screens generated by ProUCL 5.1. ProUCL 5.1 uses a pull-down menu structure, similar to a typical Windows program. For modules where no changes have been made in ProUCL since 2010 (e.g., **Sample Sizes**), screen shots as used in ProUCL 5.0 documents have been used in ProUCL 5.1 documents. Some of the screen shots generated using ProUCL 5.1 might have ProUCL 5.0 in their titles as those screen shots have not been re-generated and replaced. The screen shown below appears when the program is executed.



The above screen consists of three main window panels:

- The **MAIN WINDOW** displays data sheets and outputs results from the procedure used.
- The **NAVIGATION PANEL** displays the name of data sets and all generated outputs.
    - The navigation panel can hold up to 40 output files. In order to see more files (data files or generated output files), one can click on Widow Option.
    - In the **NAVIGATION PANEL**, ProUCL assigns self explanatory names to output files generated using the various modules of ProUCL. If the same module (e.g., **Time Series Plot**) is used many times, ProUCL identifies them by using letters a, b, c,...and so on as shown below.

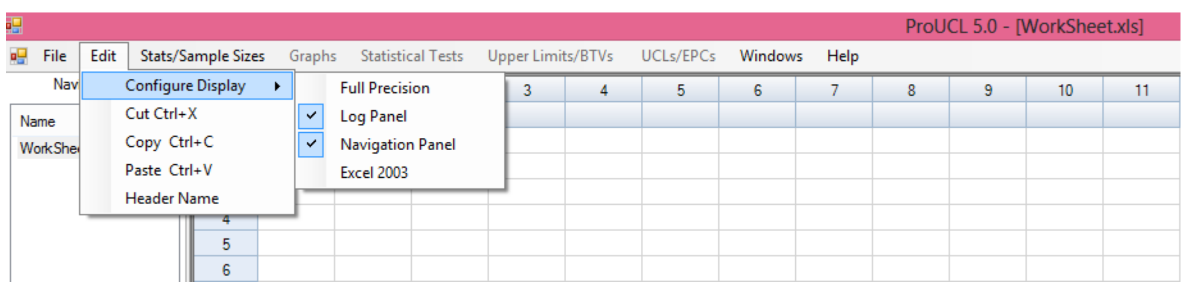


- The user may want to assign names of his choice to these output files when saving them using the "Save" or "Save As" Options.

- The **LOG PANEL** displays transactions in green, warning messages in orange, and errors in red. For an example, when one attempts to run a procedure meant for left-censored data sets on a full-uncensored data set, ProUCL 5.1 will output a warning in orange in this panel.

  - Should both panels be unnecessary, you can choose **Configure ► Panel ON/OFF**.

The use of this option gives extra space to see and print out the statistics of interest. For example, one may want to turn off these panels when multiple variables (e.g., multiple quantile-quantile [Q-Q] plots) are analyzed and goodness-of-fit (GOF) statistics and other statistics may need to be captured for all of the selected variables. The following screen was generated using ProUCL 5.0. An identical screen will be generated using ProUCL 5.1 with title name as ProUCL 5.1 - [WorkSheet.xls].



EXECUTIVE SUMMARY

The main objective of the ProUCL software funded by the United States Environmental Protection Agency (EPA) is to compute rigorous statistics to help decision makers and project teams in making good decisions at a polluted site which are cost-effective, and protective of human health and the environment. The ProUCL software is based upon the philosophy that rigorous statistical methods can be used to compute reliable estimates of population parameters and decision making statistics including: the upper confidence limit (UCL) of the mean, the upper tolerance limit (UTL), and the upper prediction limit (UPL) to help decision makers and project teams in making correct decisions. A few commonly used text book type methods (e.g., Central Limit Theorem [CLT], Student's t-UCL) alone cannot address all scenarios and situations occurring in environmental studies. Since many environmental decisions are based upon a 95 percent (%) UCL (UCL95) of the population mean, it is important to compute UCLs of practical merit. The use and applicability of a statistical method (e.g., student's t-UCL, CLT-UCL, adjusted gamma-UCL, Chebyshev UCL, bootstrap-t UCL) depend upon data size, data skewness, and data distribution. ProUCL computes decision statistics using several parametric and nonparametric methods covering a wide-range of data variability, distribution, skewness, and sample size. It is anticipated that the availability of the statistical methods in the ProUCL software covering a wide range of environmental data sets will help the decision makers in making more informative and correct decisions at Superfund and Resource Conservation and Recovery Act (RCRA) sites.

It is noted that for moderately skewed to highly skewed environmental data sets, UCLs based on the CLT and the Student's t-statistic fail to provide the desired coverage (e.g., 0.95) to the population mean even when the sample sizes are as large as 100 or more. The sample size requirements associated with the CLT increases with skewness. It would be incorrect to state that a CLT or Student's statistic based UCLs are adequate to estimate Exposure Point Concentrations (EPC) terms based upon skewed data sets. These facts have been described in the published documents (Singh, Singh, and Engelhardt [1997, 1999]; Singh, Singh, and Iaci 2002; Singh and Singh 2003; and Singh *et al.* 2006) summarizing simulation experiments conducted on positively skewed data sets to evaluate the performances of the various UCL computation methods. The use of a parametric lognormal distribution on a lognormally distributed data set yields unstable impractically large UCLs values, especially when the standard deviation (*sd*) of the log-transformed data becomes greater than 1.0 and the data set is of small size less than (<) 30-50. Many environmental data sets can be modeled by a gamma as well as a lognormal distribution. The use of a gamma distribution on gamma distributed data sets tends to yield UCL values of practical merit. Therefore, the use of gamma distribution based decision statistics such as UCLs, UPLs, and UTLs should not be dismissed by stating that it is easier to use a lognormal model to compute these upper limits.

The suggestions made in ProUCL are based upon the extensive experience of the developers in environmental statistical methods, published environmental literature, and procedures described in many EPA guidance documents. These suggestions are made to help the users in selecting the most appropriate UCL to estimate the EPC term which is routinely used in exposure assessment and risk management studies of the USEPA. The suggestions are based upon the findings of many simulation studies described in Singh, Singh, and Engelhardt (1997, 1999); Singh, Singh, and Iaci (2002); Singh and Singh (2003); and Singh *et al.* (2006). It should be pointed out that a typical simulation study does not (cannot) cover all real world data sets of various sizes and skewness from all distributions. When deemed necessary, the user may want to consult a statistician to select an appropriate upper limit to estimate the EPC term and other environmental parameters of interest. For an analyte (data set) with skewness (*sd* of logged data) near the end points of the skewness intervals presented in decision tables of Chapter 2 (e.g., Tables 2-9 through 2-11), the user may select the most appropriate UCL based upon the site conceptual site model (CSM), expert site knowledge, toxicity of the analyte, and exposure risks associated with that analyte.

The inclusion of outliers in the computation of the various decision statistics tends to yield inflated values of those decision statistics, which can lead to poor decisions. Often statistics that are computed for a data set which includes a few outliers tend to be inflated and represent those outliers rather than representing the main dominant population of interest (e.g., reference area). Identification of outliers, observations coming from population(s) other than the main dominant population is suggested, before computing the decision statistics needed to address project objectives. The project team may want to perform the statistical evaluations twice, once with outliers and once without outliers. This exercise will help the project team in computing reliable and defensible decision statistics which are needed to make cleanup and remediation decisions at polluted sites.

The initial development during 1999-2000 and all subsequent upgrades and enhancements of the ProUCL software have been funded by U.S. EPA through its Office of Research and Development (ORD). Initially ProUCL was developed as a research tool for U.S. EPA scientists and researchers of the Technical Support Center (TSC) and ORD- National Exposure Research Laboratory (NERL), Las Vegas. Background evaluations, groundwater (GW) monitoring, exposure and risk management and cleanup decisions in support of the Comprehensive Environmental Recovery, Compensation, and Liability Act (CERCLA) and RCRA site projects of the U.S. EPA are often derived based upon test statistics such as the Shapiro-Wilk (S-W) test, t-test, Wilcoxon-Mann-Whitney (WMW) test, analysis of variance (ANOVA), and Mann-Kendall (MK) test and decision statistics including UCLs of the mean, UPLs, and UTLs. To address the statistical needs of the environmental projects of the USEPA, over the years ProUCL software has been upgraded and enhanced to include many graphical tools and statistical methods described in many EPA guidance documents including: EPA 1989a, 1989b, 1991, 1992a, 1992b, 2000 Multi-Agency Radiation Survey and Site Investigation Manual (MARSSIM), 2002a, 2002b, 2002c, 2006a, 2006b, and 2009. Several statistically rigorous methods (e.g., for data sets with nondetects [NDs]) not easily available in the existing guidance documents and in the environmental literature are also available in ProUCL 5.0/ProUCL 5.1.

ProUCL 5.1/ProUCL 5.0 has graphical, estimation, and hypotheses testing methods for uncensored-full data sets and for left-censored data sets including ND observations with multiple detection limits (DLs) or reporting limits (RLs). In addition to computing general statistics, ProUCL 5.1 has goodness-of-fit (GOF) tests for normal, lognormal and gamma distributions, and parametric and nonparametric methods including bootstrap methods for skewed data sets for computation of decision making statistics such as UCLs of the mean (EPA 2002a), percentiles, UPLs for a pre-specified number of future observations (e.g., k with k=1, 2, 3,...), UPLs for mean of future k ($\geq$1) observations, and UTLs (e.g., EPA 1992b, 2002b, and 2009). Many positively skewed environmental data sets can be modeled by a lognormal as well as a gamma model. It is well-known that for moderately skewed to highly skewed data sets, the use of a lognormal distribution tends to yield inflated and unrealistically large values of the decision statistics especially when the sample size is small (e.g., <20-30). For gamma distributed skewed uncensored and left-censored data sets, ProUCL software computes decision statistics including UCLs, percentiles, UPLs for future k ($\geq$1) observations, UTLs, and upper simultaneous limits (USLs).

For data sets with NDs, ProUCL has several estimation methods including the Kaplan-Meier (KM) method, regression on order statistics (ROS) methods and substitution methods (e.g., replacing NDs by DL, DL/2). ProUCL 5.1 can be used to compute upper limits which adjust for data skewness; specifically, for skewed data sets, ProUCL computes upper limits using KM estimates in gamma (lognormal) UCL and UTL equations provided the detected observations in the left-censored data set follow a gamma (lognormal) distribution. Some poor performing commonly used and cited methods such as the DL/2 substitution method and H-statistic based UCL computation method have been retained in ProUCL 5.1 for historical reasons, and research and comparison purposes.

The **Sample Sizes** module of ProUCL can be used to develop data quality objectives (DQOs) based sampling designs and to perform power evaluations needed to address statistical issues associated with a variety of site projects. ProUCL provides user-friendly options to enter the desired values for the decision parameters such as Type I and Type II error rates, and other DQOs used to determine the minimum sample sizes needed to address project objectives. The **Sample Sizes** module can compute DQO-based minimum sample sizes needed: to estimate the population mean; to perform single and two-sample hypotheses testing approaches; and in acceptance sampling to accept or reject a batch of discrete items such as a lot of drums containing hazardous waste. Both parametric (e.g., t-test) and nonparametric (e.g., Sign test, WMW test, test for proportions) sample size determination methods are available in ProUCL.

ProUCL has exploratory graphical methods for both uncensored data sets and for left-censored data sets consisting of ND observations. Graphical methods in ProUCL include histograms, multiple quantile-quantile (Q-Q) plots, and side-by-side box plots. The use of graphical displays provides additional insight about the information contained in a data set that may not otherwise be revealed by the use of estimates (e.g., 95% upper limits) and test statistics (e.g., two-sample t-test, WMW test). In addition to providing information about the data distributions (e.g., normal or gamma), Q-Q plots are also useful in identifying outliers and the presence of mixture populations (e.g., data from several populations) potentially present in a data set. Side-by-side box plots and multiple Q-Q plots are useful to visually compare two or more data sets, such as: site-versus-background concentrations, surface-versus-subsurface concentrations, and constituent concentrations of several GW monitoring wells (MWs). ProUCL also has a couple of classical outlier test procedures, such as the Dixon test and the Rosner test which can be used on uncensored data sets as well as on left-censored data sets containing ND observations.

ProUCL has parametric and nonparametric single-sample and two-sample hypotheses testing approaches for uncensored as well as left-censored data sets. Single-sample hypotheses tests: Student's t-test, Sign test, Wilcoxon Signed Rank test, and the Proportion test are used to compare site mean/median concentrations (or some other threshold such as an upper percentile) with some average cleanup standard, C_s (or a not-to-exceed compliance limit, A_0) to verify the attainment of cleanup levels (EPA, 1989a; 2000, 2006a) at remediated site areas of concern. Single-sample tests such as the Sign test and Proportion test, and upper limits including UTLs and UPLs are also used to perform intra-well comparisons. Several two-sample hypotheses tests as described in EPA guidance documents (e.g., 2002b, 2006b, 2009) are also available in the ProUCL software. The two-sample hypotheses testing approaches in ProUCL include: Student's t-test, WMW test, Gehan test and Tarone-Ware (T-W) test. The two-sample tests are used to compare concentrations of two populations such as site versus background, surface versus subsurface soils, and upgradient versus downgradient wells.

The **Oneway ANOVA** module in ProUCL has both classical and nonparametric Kruskal-Wallis (K-W) tests. Oneway ANOVA is used to compare means (or medians) of multiple groups such as comparing mean concentrations of areas of concern and to perform inter-well comparisons. In GW monitoring applications, the ordinary least squares (OLS) regression model, trend tests, and time series plots are used to identify upwards or downwards trends potentially present in constituent concentrations identified in wells over a certain period of time. The **Trend Analysis** module performs the M-K trend test and Theil-Sen (T-S) trend test on data sets with missing values; and generates trend graphs displaying a parametric OLS regression line and nonparametric T-S trend line. The **Time Series Plots** option can be used to compare multiple time-series data sets.

The use of the incremental sampling methodology (ISM) has been recommended by the Interstate Technology and Regulatory Council (ITRC 2012) for collecting ISM soil samples to compute mean concentrations of the decision units (DUs) and sampling units (SUs) requiring characterization and remediation activities. At many polluted sites, a large amount of discrete onsite and/or offsite background data are already available which cannot be directly compared with newly collected ISM data. In order to provide a tool to compare the existing discrete background data with actual field onsite or background ISM data, a Monte Carlo Background Incremental Sample Simulator (BISS) module was incorporated in ProUCL 5.0 and retained in ProUCL 5.1 (currently blocked from general use) which may be used on a large existing discrete background data set. The BISS module simulates incremental sampling methodology based equivalent background incremental samples. The availability of a large discrete background data set collected from areas with geological conditions comparable to the DU(s) of interest is a pre-requisite for successful application of this module. For now, the BISS module has been blocked for use as this module is awaiting adequate guidance and instructions for its intended use on discrete background data sets.

ProUCL software is a user-friendly freeware package providing statistical and graphical tools needed to address statistical issues described in many U.S. EPA guidance documents. ProUCL 5.0/ProUCL 5.1 can process many constituents (variables) simultaneously to: perform statistical tests (e.g., ANOVA and trend test statistics) and compute decision statistics including UCLs of mean, UPLs, and UTLs – a capability not available in several commercial software packages such as Minitab 16 and NADA for R (Helsel 2013). ProUCL also has the capability of processing data by group variables. Special care has been taken to make the software as user friendly as possible. For example, on the various GOF graphical displays, output sheets for GOF tests, OLS and ANOVA, in addition to critical values and/or p-values, the conclusion derived based upon those values is also displayed. ProUCL is easy to use and does not require any programming skills as needed when using commercial software packages and programs written in R script.

Methods incorporated in ProUCL have been tested and verified extensively by the developers, researchers, scientists, and users. The results obtained by ProUCL are in agreement with the results obtained by using other software packages including Minitab, SAS®, and programs written in R Script. ProUCL 5.0/ProUCL 5.1 computes decision statistics (e.g., UPL, UTL) based upon the KM method in a straight forward manner without flipping the data and re-flipping the computed statistics for left-censored data sets; these operations are not easy for a typical user to understand and perform. This can become unnecessarily tedious when computing decision statistics for multiple variables/analytes. Moreover, unlike survival analysis, it is important to compute an accurate estimate of the *sd* which is needed to compute decision making statistics including UPLs and UTLs. For left-censored data sets, ProUCL computes a KM estimate of *sd* directly. These issues are elaborated by examples discussed in this User Guide and in the accompanying ProUCL 5.1 Technical Guide.

ProUCL does not represent a policy software of the government. ProUCL has been developed on limited resources, and it does provide many statistical methods often used in environmental applications. The objective of the freely available user-friendly software, ProUCL is to provide statistical and graphical tools to address environmental issues of environmental site projects for all *users* including those users who cannot or may not want to program and/or do not have access to commercial software packages. Some users have criticized ProUCL and pointed out some deficiencies such as: it does not have geostatistical methods; it does not perform simulations; and does not offer programming interface for automation. Due to the limited scope of ProUCL, advanced methods have not been incorporated in ProUCL. For methods not available in ProUCL, users can use other statistical software packages such as SAS® (available to EPA personnel) and R script to address their computational needs. Contributions from scientists and researchers to enhance methods incorporated in ProUCL will be very much appreciated. Just like other government documents (e.g., U.S. EPA 2009), various versions of ProUCL (2007, 2009, 2011, 2013, 2016) also make some rule-of thumb type suggestions (e.g., minimum sample size requirement of 8-10) based upon professional judgment and experience of the developers. It is recommended that the users/project team/agencies make their own determinations about the rule-of-thumb type suggestions made in ProUCL before applying a statistical method.

ACRONYMS and ABBREVIATIONS

ACL	Alternative compliance or concentration limit
A-D, AD	Anderson-Darling test
AL	Action limit
AOC	Area(s) of concern
ANOVA	Analysis of variance
A_0	Not to exceed compliance limit or specified action level
BC	Box-Cox transformation
BCA	Bias-corrected accelerated bootstrap method
BD	Binomial distribution
BISS	Background Incremental Sample Simulator
BTV	Background threshold value
CC, cc	Confidence coefficient
CERCLA	Comprehensive Environmental Recovery, Compensation, and Liability Act
CL	Compliance limit
CLT	Central Limit Theorem
COPC	Contaminant/constituent of potential concern
C_s	Cleanup standards
CSM	Conceptual site model
Df	Degrees of freedom
DL	Detection limit
DL/2 (t)	UCL based upon DL/2 method using Student's t-distribution cutoff value
DL/2 Estimates	Estimates based upon data set with NDs replaced by 1/2 of the respective detection limits
DOE	Department of Energy
DQOs	Data quality objectives
DU	Decision unit
EA	Exposure area
EDF	Empirical distribution function
EM	Expectation maximization
EPA	United States Environmental Protection Agency

EPC	Exposure point concentration
GA	Georgia
GB	Gigabyte
GHz	Gigahertz
GROS	Gamma ROS
GOF, G.O.F.	Goodness-of-fit
GUI	Graphical user interface
GW	Groundwater
H_A	Alternative hypothesis
H_0	Null hypothesis
H-UCL	UCL based upon Land's H-statistic
i.i.d.	Independently and identically distributed
ISM	Incremental sampling methodology
ITRC	Interstate Technology & Regulatory Council
k, K	Positive integer representing future or next k observations
K	Shape parameter of a gamma distribution
K,k	Number of nondetects in a data set
k hat	MLE of the shape parameter of a gamma distribution
k star	Biased corrected MLE of the shape parameter of a gamma distribution
KM (%)	UCL based upon Kaplan-Meier estimates using the percentile bootstrap method
KM (Chebyshev)	UCL based upon Kaplan-Meier estimates using the Chebyshev inequality
KM (t)	UCL based upon Kaplan-Meier estimates using the Student's t-distribution critical value
KM (z)	UCL based upon Kaplan-Meier estimates using critical value of a standard normal distribution
K-M, KM	Kaplan-Meier
K-S, KS	Kolmogorov-Smirnov
K-W	Kruskal Wallis
LCL	Lower confidence limit
LN, *ln*	Lognormal distribution
LCL	Lower confidence limit of mean
LPL	Lower prediction limit
LROS	LogROS; robust ROS

LTL	Lower tolerance limit
LSL	Lower simultaneous limit
M,m	Applied to incremental sampling: number in increments in an ISM sample
MARSSIM	Multi-Agency Radiation Survey and Site Investigation Manual
MCL	Maximum concentration limit, maximum compliance limit
MDD	Minimum detectable difference
MDL	Method detection limit
MK, M-K	Mann-Kendall
ML	Maximum likelihood
MLE	Maximum likelihood estimate
n	Number of observations/measurements in a sample
N	Number of observations/measurements in a population
MVUE	Minimum variance unbiased estimate
MW	Monitoring well
NARPM	National Association of Remedial Project Managers
ND, nd, Nd	Nondetect
NERL	National Exposure Research Laboratory
NRC	Nuclear Regulatory Commission
OKG	Orthogonalized Kettenring Gnanadesikan
OLS	Ordinary least squares
ORD	Office of Research and Development
OSRTI	Office of Superfund Remediation and Technology Innovation
OU	Operating unit
PCA	Principal component analysis
PDF, pdf	Probability density function
.pdf	Files in Portable Document Format
PRG	Preliminary remediation goals
PROP	Proposed influence function
p-values	Probability-values
QA	Quality assurance
QC	Quality
Q-Q	Quantile-quantile

R,r	Applied to incremental sampling: number of replicates of ISM samples
RAGS	Risk Assessment Guidance for Superfund
RCRA	Resource Conservation and Recovery Act
RL	Reporting limit
RMLE	Restricted maximum likelihood estimate
ROS	Regression on order statistics
RPM	Remedial Project Manager
RSD	Relative standard deviation
RV	Random variable
S	Substantial difference
SCMTSC	Site Characterization and Monitoring Technical Support Center
SD, *Sd, sd*	Standard deviation
SE	Standard error
SND	Standard Normal Distribution
SNV	Standard Normal Variate
SSL	Soil screening levels
SQL	Sample quantitation limit
SU	Sampling unit
S-W, SW	Shapiro-Wilk
T-S	Theil-Sen
TSC	Technical Support Center
TW, T-W	Tarone-Ware
UCL	Upper confidence limit
UCL95	95% upper confidence limit
UPL	Upper prediction limit
U.S. EPA, EPA	United States Environmental Protection Agency
UTL	Upper tolerance limit
UTL95-95	95% upper tolerance limit with 95% coverage
USGS	U.S. Geological Survey
USL	Upper simultaneous limit
vs.	Versus
WMW	Wilcoxon-Mann-Whitney

WRS	Wilcoxon Rank Sum
WSR	Wilcoxon Signed Rank
X_p	p^{th} percentile of a distribution
$<$	Less than
$>$	Greater than
$\geq$	Greater than or equal to
$\leq$	Less than or equal to
Δ	Greek letter denoting the width of the gray region associated with hypothesis testing
Σ	Greek letter representing the summation of several mathematical quantities, numbers
%	Percent
α	Type I error rate
β	Type II error rate
Θ	Scale parameter of the gamma distribution
Σ	Standard deviation of the log-transformed data
^	carat sign over a parameter, indicates that it represents a statistic/estimate computed using the sampled data

GLOSSARY

Anderson-Darling (A-D) test: The Anderson-Darling test assesses whether known data come from a specified distribution. In ProUCL the A-D test is used to test the null hypothesis that a sample data set, x_1, ..., x_n came from a gamma distributed population.

Background Measurements: Measurements that are not site-related or impacted by site activities. Background sources can be naturally occurring or anthropogenic (man-made).

Bias: The systematic or persistent distortion of a measured value from its true value (this can occur during sampling design, the sampling process, or laboratory analysis).

Bootstrap Method: The bootstrap method is a computer-based method for assigning measures of accuracy to sample estimates. This technique allows estimation of the sample distribution of almost any statistic using only very simple methods. Bootstrap methods are generally superior to ANOVA for small data sets or where sample distributions are non-normal.

Central Limit Theorem (CLT): The central limit theorem states that given a distribution with a mean, μ, and variance, σ^2, the sampling distribution of the mean approaches a normal distribution with a mean (μ) and a variance σ^2/N as N, the sample size, increases.

Censored Data Sets: Data sets that contain one or more observations which are nondetects.

Coefficient of Variation (CV): A dimensionless quantity used to measure the spread of data relative to the size of the numbers. For a normal distribution, the coefficient of variation is given by s/xBar. It is also known as the relative standard deviation (RSD).

Confidence Coefficient (CC): The confidence coefficient (a number in the closed interval [0, 1]) associated with a confidence interval for a population parameter is the probability that the random interval constructed from a random sample (data set) contains the true value of the parameter. The confidence coefficient is related to the significance level of an associated hypothesis test by the equality: level of significance = 1 – confidence coefficient.

Confidence Interval: Based upon the sampled data set, a confidence interval for a parameter is a random interval within which the unknown population parameter, such as the mean, or a future observation, x_0, falls.

Confidence Limit: The lower or an upper boundary of a confidence interval. For example, the 95% upper confidence limit (UCL) is given by the upper bound of the associated confidence interval.

Coverage, Coverage Probability: The coverage probability (e.g., = 0.95) of an upper confidence limit (UCL) of the population mean represents the confidence coefficient associated with the UCL.

Critical Value: The critical value for a hypothesis test is a threshold to which the value of the test statistic is compared to determine whether or not the null hypothesis is rejected. The critical value for any hypothesis test depends on the sample size, the significance level, α at which the test is carried out, and whether the test is one-sided or two-sided.

Data Quality Objectives (DQOs): Qualitative and quantitative statements derived from the DQO process that clarify study technical and quality objectives, define the appropriate type of data, and specify tolerable levels of potential decision errors that will be used as the basis for establishing the quality and quantity of data needed to support decisions.

Detection Limit: A measure of the capability of an analytical method to distinguish samples that do not contain a specific analyte from samples that contain low concentrations of the analyte. It is the lowest concentration or amount of the target analyte that can be determined to be different from zero by a single measurement at a stated level of probability. Detection limits are analyte and matrix-specific and may be laboratory-dependent.

Empirical Distribution Function (EDF): In statistics, an empirical distribution function is a cumulative probability distribution function that concentrates probability $1/n$ at each of the n numbers in a sample.

Estimate: A numerical value computed using a random data set (sample), and is used to guess (estimate) the population parameter of interest (e.g., mean). For example, a sample mean represents an estimate of the unknown population mean.

Expectation Maximization (EM): The EM algorithm is used to approximate a probability density function (PDF). EM is typically used to compute maximum likelihood estimates given incomplete samples.

Exposure Point Concentration (EPC): The constituent concentration within an exposure unit to which the receptors are exposed. Estimates of the EPC represent the concentration term used in exposure assessment.

Extreme Values: Values that are well-separated from the majority of the data set coming from the far/extreme tails of the data distribution.

Goodness-of-Fit (GOF): In general, the level of agreement between an observed set of values and a set wholly or partly derived from a model of the data.

Gray Region: A range of values of the population parameter of interest (such as mean constituent concentration) within which the consequences of making a decision error are relatively minor. The gray region is bounded on one side by the action level. The width of the gray region is denoted by the Greek letter delta, Δ, in this guidance.

H-Statistic: Land's statistic used to compute UCL of mean of a lognormal population

H-UCL: UCL based on Land's H-Statistic.

Hypothesis: Hypothesis is a statement about the population parameter(s) that may be supported or rejected by examining the data set collected for this purpose. There are two hypotheses: a null hypothesis, (H_0), representing a testable presumption (often set up to be rejected based upon the sampled data), and an alternative hypothesis (H_A), representing the logical opposite of the null hypothesis.

Jackknife Method: A statistical procedure in which, in its simplest form, estimates are formed of a parameter based on a set of N observations by deleting each observation in turn to obtain, in addition to the usual estimate based on N observations, N estimates each based on N-1 observations.

Kolmogorov-Smirnov (KS) test: The Kolmogorov-Smirnov test is used to decide if a data set comes from a population with a specific distribution. The Kolmogorov-Smirnov test is based on the empirical distribution function (EDF). ProUCL uses the KS test to test the null hypothesis if a data set follows a gamma distribution.

Left-censored Data Set: An observation is left-censored when it is below a certain value (detection limit) but it is unknown by how much; left-censored observations are also called nondetect (ND) observations. A data set consisting of left-censored observations is called a left-censored data set. In environmental applications trace concentrations of chemicals may indeed be present in an environmental sample (e.g., groundwater, soil, sediment) but cannot be detected and are reported as less than the detection limit of the analytical instrument or laboratory method used.

Level of Significance (α): The error probability (also known as false positive error rate) tolerated of falsely rejecting the null hypothesis and accepting the alternative hypothesis.

Lilliefors test: A goodness-of-fit test that tests for normality of large data sets when population mean and variance are unknown.

Maximum Likelihood Estimates (MLE): MLE is a popular statistical method used to make inferences about parameters of the underlying probability distribution of a given data set.

Mean: The sum of all the values of a set of measurements divided by the number of values in the set; a measure of central tendency.

Median: The middle value for an ordered set of n values. It is represented by the central value when n is odd or by the average of the two most central values when n is even. The median is the 50th percentile.

Minimum Detectable Difference (MDD): The MDD is the smallest difference in means that the statistical test can resolve. The MDD depends on sample-to-sample variability, the number of samples, and the power of the statistical test.

Minimum Variance Unbiased Estimates (MVUE): A minimum variance unbiased estimator (MVUE or MVU estimator) is an unbiased estimator of parameters, whose variance is minimized for all values of the parameters. If an estimator is unbiased, then its mean squared error is equal to its variance.

Nondetect (ND) values: Censored data values. Typically, in environmental applications, concentrations or measurements that are less than the analytical/instrument method detection limit or reporting limit.

Nonparametric: A term describing statistical methods that do not assume a particular population probability distribution, and are therefore valid for data from any population with any probability distribution, which can remain unknown.

Optimum: An interval is optimum if it possesses optimal properties as defined in the statistical literature. This may mean that it is the shortest interval providing the specified coverage (e.g., 0.95) to the population mean. For example, for normally distributed data sets, the UCL of the population mean based upon Student's t distribution is optimum.

Outlier: Measurements (usually larger or smaller than the majority of the data values in a sample) that are not representative of the population from which they were drawn. The presence of outliers distorts most statistics if used in any calculations.

Probability - Values (*p*-value): In statistical hypothesis testing, the p-value associated with an observed value, t_{observed} of some random variable T used as a test statistic is the probability that, given that the null hypothesis is true, T will assume a value as or more unfavorable to the null hypothesis as the observed value t_{observed}. The null hypothesis is rejected for all levels of significance, α greater than or equal to the p-value.

Parameter: A parameter is an unknown or known constant associated with the distribution used to model the population.

Parametric: A term describing statistical methods that assume a probability distribution such as a normal, lognormal, or a gamma distribution.

Population: The total collection of N objects, media, or people to be studied and from which a sample is to be drawn. It is the totality of items or units under consideration.

Prediction Interval: The interval (based upon historical data, background data) within which a newly and independently obtained (often labeled as a future observation) site observation (e.g., onsite, compliance well) of the predicted variable (e.g., lead) falls with a given probability (or confidence coefficient).

Probability of Type II (2) Error (β): The probability, referred to as β (beta), that the null hypothesis will not be rejected when in fact it is false (false negative).

Probability of Type I (1) Error = Level of Significance (α): The probability, referred to as α (alpha), that the null hypothesis will be rejected when in fact it is true (false positive).

pth Percentile or pth Quantile: The specific value, X_p of a distribution that partitions a data set of measurements in such a way that the p percent (a number between 0 and 100) of the measurements fall at or below this value, and (100-p) percent of the measurements exceed this value, X_p.

Quality Assurance (QA): An integrated system of management activities involving planning, implementation, assessment, reporting, and quality improvement to ensure that a process, item, or service is of the type and quality needed and expected by the client.

Quality Assurance Project Plan: A formal document describing, in comprehensive detail, the necessary QA, quality control (QC), and other technical activities that must be implemented to ensure that the results of the work performed will satisfy the stated performance criteria.

Quantile Plot: A graph that displays the entire distribution of a data set, ranging from the lowest to the highest value. The vertical axis represents the measured concentrations, and the horizontal axis is used to plot the percentiles/quantiles of the distribution.

Range: The numerical difference between the minimum and maximum of a set of values.

Regression on Order Statistics (ROS): A regression line is fit to the normal scores of the order statistics for the uncensored observations and is used to fill in values imputed from the straight line for the observations below the detection limit.

Resampling: The repeated process of obtaining representative samples and/or measurements of a population of interest.

Reliable UCL: see Stable UCL.

Robustness: Robustness is used to compare statistical tests. A robust test is the one with good performance (that is not unduly affected by outliers and underlying assumptions) for a wide variety of data distributions.

Resistant Estimate: A test/estimate which is not affected by outliers is called a resistant test/estimate

Sample: Represents a random sample (data set) obtained from the population of interest (e.g., a site area, a reference area, or a monitoring well). The sample is supposed to be a representative sample of the population under study. The sample is used to draw inferences about the population parameter(s).

Shapiro-Wilk (SW) test: Shapiro-Wilk test is a goodness-of-fit test that tests the null hypothesis that a sample data set, $x_1, ..., x_n$ came from a normally distributed population.

Skewness: A measure of asymmetry of the distribution of the parameter under study (e.g., lead concentrations). It can also be measured in terms of the standard deviation of log-transformed data. The greater the standard deviation, the greater is the skewness.

Stable UCL: The UCL of a population mean is a stable UCL if it represents a number of practical merit (e.g., a realistic value which can actually occur at a site), which also has some physical meaning. That is, a stable UCL represents a realistic number (e.g., constituent concentration) that can occur in practice. Also, a stable UCL provides the specified (at least approximately, as much as possible, as close as possible to the specified value) coverage (e.g., ~0.95) to the population mean.

Standard Deviation (*sd*, sd, SD): A measure of variation (or spread) from an average value of the sample data values.

Standard Error (SE): A measure of an estimate's variability (or precision). The greater the standard error in relation to the size of the estimate, the less reliable is the estimate. Standard errors are needed to construct confidence intervals for the parameters of interests such as the population mean and population percentiles.

Substitution Method: The substitution method is a method for handling NDs in a data set, where the ND is replaced by a defined value such as 0, DL/2 or DL prior to statistical calculations or graphical analyses. This method has been included in ProUCL 5.1 for historical comparative purposes but **is not recommended** for use. The **bias** introduced by applying the substitution method **cannot be quantified** with any certainty. ProUCL 5.1 will provide a warning when this option is chosen.

Uncensored Data Set: A data set without any censored (nondetects) observations.

Unreliable UCL, Unstable UCL, Unrealistic UCL: The UCL of a population mean is unstable, unrealistic, or unreliable if it is orders of magnitude higher than the other UCLs of a population mean. It represents an impractically large value that cannot be achieved in practice. For example, the use of Land's H-statistic often results in an impractically large inflated UCL value. Some other UCLs, such as the bootstrap-t UCL and Hall's UCL, can be inflated by outliers resulting in an impractically large and unstable value. All such impractically large UCL values are called unstable, unrealistic, unreliable, or inflated UCLs.

Upper Confidence Limit (UCL): The upper boundary (or limit) of a confidence interval of a parameter of interest such as the population mean.

Upper Prediction Limit (UPL): The upper boundary of a prediction interval for an independently obtained observation (or an independent future observation).

Upper Tolerance Limit (UTL): A confidence limit on a percentile of the population rather than a confidence limit on the mean. For example, a 95% one-sided UTL for 95% coverage represents the value below which 95% of the population values are expected to fall with 95 % confidence. In other words, a 95% UTL with coverage coefficient 95% represents a 95% UCL for the 95th percentile.

Upper Simultaneous Limit (USL): The upper boundary of the largest value.

xBar: arithmetic average of computed using the sampled data values

ACKNOWLEDGEMENTS

We wish to express our gratitude and thanks to our friends and colleagues who have contributed during the development of past versions of ProUCL and to all of the many people who reviewed, tested, and gave helpful suggestions throughout the development of the ProUCL software package. We wish to especially acknowledge EPA scientists including Deana Crumbling, Nancy Rios-Jafolla, Tim Frederick, Dr. Maliha Nash, Kira Lynch, and Marc Stiffleman; James Durant of ATSDR, Dr. Steve Roberts of University of Florida, Dr. Elise A. Striz of the National Regulatory Commission (NRC), and Drs. Phillip Goodrum and John Samuelian of Integral Consulting Inc. for testing and reviewing ProUCL 5.0 and its associated guidance documents, and for providing helpful comments and suggestions. We also wish to thank Dr. D. Beal of Leidos for reviewing ProUCL 5.0.

Special thanks go to Ms. Donna Getty and Mr. Richard Leuser of Lockheed Martin for providing a thorough technical and editorial review of ProUCL 5.1 and also ProUCL 5.0 User Guide and Technical Guide. A special note of thanks is due to Ms. Felicia Barnett of EPA ORD Site Characterization and Monitoring Technical Support Center (SCMTSC), without whose assistance the development of the ProUCL 5.1 software and associated guidance documents would not have been possible.

Finally, we wish to dedicate the ProUCL 5.1 (and ProUCL 5.0) software package to our friend and colleague, John M. Nocerino who had contributed significantly in the development of ProUCL and Scout software packages.

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INTRODUCTION

OVERVIEW OF ProUCL VERSION 5.1 SOFTWARE

The main objective of the ProUCL software funded by the U.S.EPA is to compute rigorous decision statistics to help the decision makers in making reliable decisions which are cost-effective, and protective of human health and the environment. The development of ProUCL software is based upon the philosophy that rigorous statistical methods can be used to compute representative estimates of population parameters (e.g., site mean, background percentiles) and accurate decision making statistics (including the upper confidence limit [UCL] of the mean, upper tolerance limit [UTL], and upper prediction limit [UPL]) which will assist decision makers and project teams in making sound decisions. The use and applicability of a statistical method (e.g., student's t-UCL, Central Limit Theorem (CLT)-UCL, adjusted gamma-UCL, Chebyshev UCL, bootstrap-t UCL) depend upon data size, data variability, data skewness, and data distribution. ProUCL computes decision statistics using several parametric and nonparametric methods covering a wide-range of data variability, skewness, and sample size. A couple of text book methods described in most of the statistical text books (e.g., Hogg and Craig, 1995) based upon the Student's t-statistic and the CLT alone cannot address all scenarios and situations commonly occurring in environmental studies. It is incorrect to assume that Student's t-statistic and/or CLT based UCLs of mean will provide the desired coverage (e.g., 0.95) to the population mean irrespective of the skewness of the data set/population under consideration. These issues have been discussed in detail in Chapters 2 and 4 of the accompanying ProUCL 5.1 Technical Guide. Several examples are provided in the Technical Guide which elaborate on these issues.

The use of a parametric lognormal distribution on a lognormally distributed data set tends to yield unstable impractically large UCL values, especially when the standard deviation of the log-transformed data is greater than 1.0 and the data set is of small size such as less than 30-50 (Hardin and Gilbert 1993; Singh, Singh, and Engelhardt 1997). Many environmental data sets can be modeled by a gamma as well as a lognormal distribution. Generally, the use of a gamma distribution on gamma distributed data sets yields UCL values of practical merit (Singh, Singh, and Iaci 2002). Therefore, the use of gamma distribution based decision statistics such as UCLs, UPL, and UTLs cannot be dismissed just because it is easier to use a lognormal model to compute these upper limits. The two distributions do not behave in a similar manner. The advantages of computing the gamma distribution-based decision statistics are discussed in Chapters 2 through 5 of the ProUCL Technical Guide.

Since many environmental decisions are made based upon a 95% UCL of the population mean, it is important to compute reliable UCLs and other decision making statistics of practical merit. In an effort to compute stable UCLs of the population mean and other decision making statistics, in addition to computing the Student's t statistic and the CLT based statistics (e.g., UCLs, UPLs), significant effort has been made to incorporate rigorous statistical methods for computing UCLs (and other limits) in the ProUCL software, covering a wide-range of data skewness and sample sizes (e.g., Singh, Singh, and Engelhardt, 1997; Singh, Singh, and Iaci, 2002; and Singh, Singh, 2003). It is anticipated that the availability of the statistical methods in the ProUCL software, which can be applied to a wide range of environmental data sets, will help decision makers in making more informative, practical and sound decisions.

It is noted that even for skewed data sets, practitioners tend to use the CLT or Student's t-statistic based UCLs of mean for "large" sample sizes of 25-30 (rule-of-thumb to use CLT). However, this rule-of-thumb does not apply for moderately to highly skewed data sets, specifically when σ (standard deviation of the log-transformed data) starts exceeding 1. The large sample size requirement associated with the use of the CLT depends upon the skewness of the data distribution under consideration. The large sample requirement associated with CLT for the sample mean to follow an approximate normal distribution increases with the data skewness; and for highly skewed data sets, even samples of size greater than (>)100 may not be large enough for the sample mean to follow an approximate normal distribution. For moderately skewed to highly skewed environmental data sets, as expected, UCLs based on the CLT and the Student's t-statistic fail to provide the desired coverage of the population mean even when the sample sizes are as large as 100 or more. These facts have been verified in the published simulation experiments conducted on positively skewed data sets (e.g., Singh, Singh, and Engelhardt, 1997; Singh, Singh, and Iaci, 2002; and Singh and Singh, 2003); some graphs showing the simulation results are provided in Appendix B of the ProUCL 5.1 Technical Guide.

The initial development and all subsequent upgrades and enhancements of the ProUCL software have been funded by the U.S. EPA through its Office of Research and Development (ORD). Initially ProUCL was developed as a research tool for scientists and researchers of the Technical Support Center and ORD-NERL, Las Vegas. During 1999-2001, the initial intent and objectives of developing the ProUCL software (Version 1.0 and Version 2.0) were to provide a statistical research tool for EPA scientists which can be used to compute theoretically sound 95% upper confidence limits (UCL95s) of the mean routinely used in exposure assessment, risk management and cleanup decisions made at various CERCLA and RCRA sites (EPA 1992a, 2002a). During 2002, the peer-reviewed ProUCL version 2.1 (with Chebyshev inequality based UCLs) was released for public use. Several researchers have developed rigorous parametric and nonparametric statistical methods (e.g., Johnson 1978; Grice and Bain 1980; Efron [1981 1982]; Efron and Tibshirani 1993; Hall [1988, 1992]; Sutton 1993; Chen 1995; Singh, Singh, and Engelhardt 1997; Singh, Singh, and Iaci 2002] to compute upper limits (e.g., UCLs) which adjust for data skewness. Since Student's t-UCL, CLT-UCL, and percentile bootstrap UCL fail to provide the desired coverage to the population mean of skewed distributions, several parametric (e.g., gamma distribution based) and nonparametric (e.g., bias-corrected accelerated [BCA] bootstrap and bootstrap-t, Chebyshev UCL) UCL computation methods which adjust for data skewness were incorporated in ProUCL versions 3.0 and 3.00.02 during 2003-2004. ProUCL version 3.00.02 also had graphical Q-Q plots and GOF tests for normal, lognormal, and gamma distributions; capabilities to statistically analyze multiple variables simultaneously were also incorporated in ProUCL 3.00.02 (EPA 2004).

It is important to compute decision statistics (e.g., UCLs, UTLs) which are cost-effective and protective of human health and the environment (balancing between Type I and Type II errors), therefore, one cannot dismiss the use of the better [better than t-UCL, CLT-UCL, ROS and KM percentile bootstrap UCL, KM-UCL (t)] performing UCL computation methods including gamma UCLs and the various bootstrap UCLs which adjust for data skewness. During 2004-2007, ProUCL was upgraded to versions 4.00.02, and 4.00.04. These upgrades included exploratory graphical (e.g., Q-Q plots, box plots) and statistical (e.g., maximum likelihood estimation [MLE], KM, and ROS) methods for left-censored data sets consisting of nondetect (NDs) observations with multiple DLs or RLs. For uncensored and left-censored data sets, these upgrades provide statistical methods to compute upper limits: percentiles, UPLs and UTLs needed to estimate site-specific background level constituent concentrations or background threshold values (BTVs). To address statistical needs of background evaluation projects (e.g., EPA 2000, 2002b), several single-sample and two-sample hypotheses testing approaches were also included in these ProUCL upgrades.

During 2008-2010, ProUCL was upgraded to ProUCL 4.00.05. The upgraded ProUCL was enhanced by including methods to compute gamma distribution based UPLs and UTLs (Krishnamoorthy, Mathew, and Mukherjee 2008). The **Sample Size** module to compute DQOs-based minimum sample sizes, needed to address statistical issues associated with environmental projects (e.g., EPA 2000,2002c, 2006a, 2006b), was also incorporated in ProUCL 4.00.05.

During 2009-2011, ProUCL 4.00.05 was upgraded to ProUCL 4.1 and 4.1.01. ProUCL 4.1 (2010) and 4.1.01 (2011) retain all capabilities of the previous versions of ProUCL software. Two new modules: **Oneway ANOVA** and **Trend Analysis** were included in ProUCL 4.1. The **Oneway ANOVA** module has both parametric and nonparametric ANOVA tests to perform inter-well comparisons. The **Trend Analysis** module can be used to determine potential upward or downward trends present in constituent concentrations identified in GW monitoring wells (MWs). The **Trend Analysis** module can compute Mann-Kendall (MK) and Theil-Sen (T-S) trend statistics to determine upward or downward trends potentially present in analyte concentrations. ProUCL 4.1 also has the **OLS Regression** module. In ProUCL 4.1, some modifications were made in decision tables which are used to make suggestions regarding the use of UCL95 for estimating EPCs. Specifically, based upon experience, developers of ProUCL re-iterated that the use of a lognormal distribution for estimating EPCs and BTVs should be avoided, as the use of the lognormal distribution tends to yield unrealistic and unstable values of decision making statistics including UCLs, UPLs, and UTLs. This is especially true when the sample size is <20-30 and the data set is moderately to highly skewed. During March 2011, webinars were presented describing the capabilities and use of the methods available in ProUCL 4.1, which can be downloaded from the EPA ProUCL website.

ProUCL version 5.0.00 (EPA 2013, 2014) represents an upgrade of ProUCL 4.1.01 (EPA June 2011) which represents an upgrade of ProUCL 4.1.00 (EPA 2010). For uncensored and left-censored data sets, ProUCL 5.0.00 (ProUCL 5.0) contains all statistical and graphical methods that were available in the previous versions of the ProUCL software package except for some poor performing and restricted (e.g., can be used only when a single detection limit is present) estimation methods such as the MLE and winsorization methods for left-censored data sets. ProUCL has GOF tests for normal, lognormal, and gamma distributions for uncensored and left-censored data sets with NDs. ProUCL 5.0 has the extended version of the Shapiro-Wilk (S-W) test to perform normal and lognormal GOF tests for data sets of sizes up to 2000 (Royston [1982, 1982a]). In addition to normal and lognormal distribution- based decision statistics, ProUCL software computes UCLs, UPLs, and UTLs based upon the gamma distribution.

Several enhancements were made in the **UCLs/EPCs** and **Upper Limits/BTVs** modules of the ProUCL 5.0 software. A new statistic, an upper simultaneous limit (USL) (Singh and Nocerino 2002; Wilks 1963) has been incorporated in the **Upper Limits/BTVs** module of ProUCL 5.0 for data sets consisting of NDs with multiple DLs. A two-sample hypothesis test, the Tarone-Ware (T-W; Tarone and Ware, 1978) test has also been incorporated in ProUCL 5.0. Nonparametric tolerance limits have been enhanced, and for specific values of confidence coefficients, coverage probability, and sample size, ProUCL 5.0 outputs the confidence coefficient (CC) actually achieved by a UTL. The **Trend Analysis** and **OLS Regression** modules can handle missing events when computing trend test statistics and generating trend graphs. Some new methods using KM estimates in gamma (and lognormal) distribution-based UCL, UPL, and UTL equations have been incorporated to compute the decision statistics for data sets consisting of nondetect observations. To facilitate the computation of UCLs from ISM based samples (ITRC 2012); the minimum sample size requirement has been lowered to 3, so that one can compute the UCL95 based upon ISM data sets of sizes ≥3.

All known bugs, typographical errors, and discrepancies found by the developers and users of the ProUCL software package were addressed in ProUCL version 5.0.00. Specifically, a discrepancy found in the estimate of mean based upon the KM method was fixed in ProUCL 5.0. Some changes were made in the decision logic used in the **Goodness of Fit** and **UCLs/EPCs** modules. In practice, based upon a given data set, it is well known that the two statistical tests (e.g., T-S and OLS trend tests) can lead to different conclusions. To streamline the decision logic associated with the computation of the various UCLs, the decision tables in ProUCL 5.0 were updated. Specifically, for each distribution if at least one of the two GOF tests (e.g., Shapiro-Wilk or Lilliefors test for normality) determines that the hypothesized distribution holds, then ProUCL concludes that the data set follows the hypothesized distribution, and decision statistics are computed accordingly. Additionally, for gamma distributed data sets, ProUCL 5.0 suggests the use of the: adjusted gamma UCL for samples of sizes ≤ 50 (instead of 40 suggested in previous versions); and approximate gamma UCL for samples of sizes >50.

Also, for samples of larger sizes (e.g., with $n > 100$) and small values of the gamma shape parameter, k (e.g., $k \leq 0.1$), significant discrepancies were found in the critical values of the two gamma GOF test statistics (Anderson-Darling [A-D] and Kolmogorov Smirnov [K-S] tests) obtained using the two gamma deviate generation algorithms: Whitaker (1974) and Marsaglia and Tsang (2000). For values of $k \leq 0.2$, the critical values of the two gamma GOF tests: A-D and K-S tests have been updated using the currently available more accurate gamma deviate generation algorithm due to Marsaglia and Tsang's (2000); more details about the implementation of their algorithm can be found in Kroese, Taimre, and Botev (2011). For values of the shape parameter, $k=0.025, 0.05, 0.1$, and 0.2, the critical value tables for these two tests were updated by incorporating the newly generated critical values for the three significance levels: 0.05, 0.1, and 0.01. The updated tables are provided in Appendix A of the ProUCL 5.0/ProUCL 5.1 Technical Guide. It should be noted that for $k=0.2$, the older and the newly generated critical values are in general agreement; therefore, critical values for $k=0.2$ were not replaced in tables summarized in Appendix A of the ProUCL Technical Guide.

ProUCL 5.0 also has a new **Background Incremental Sample Simulator** (BISS) module (temporarily blocked for general public use) which can be used on a large existing discrete background data set to simulate background incremental samples. The availability of a large discrete data set collected from areas with geological formations and conditions comparable to the DUs (background or onsite) of interest is a requirement for successful application of this module. The simulated BISS data can be compared with the actual field ISM (ITRC 2012) data collected from the various DUs using other modules of ProUCL 5.0. The values of the BISS data are not directly available to users; however, the simulated BISS data can be accessed by the various modules of ProUCL 5.0 to perform desired statistical evaluations. For example, the simulated background BISS data can be merged with the actual field ISM data after comparing the two data sets using a two-sample t-test; the simulated BISS or the merged data can be used to compute a UCL of the mean or a UTL.

Note: The ISM methodology used to develop the **BISS** module is a relatively new approach; methods incorporated in this **BISS** module requires further investigation. For now, the **BISS** module has been blocked for use in ProUCL 5.0/ProUCL 5.1 as this module is awaiting adequate guidance and instructions for its intended use on discrete background data sets.

ProUCL 5.0 is a user-friendly freeware package providing statistical and graphical tools needed to address statistical issues described in several EPA guidance documents. Considerable effort was made to provide a detailed technical guide to help practitioners understand the statistical methods needed to address the statistical needs of their environmental projects. ProUCL generates detailed output sheets and graphical displays for each method which can be used to educate students learning environmental statistical methods. Like previous versions, ProUCL 5.0 can process many variables simultaneously to compute various tests (e.g., ANOVA and trend test statistics) and decision statistics including UCL of the mean, UPLs, and UTLs, a capability not available in other software packages such as Minitab 16 and NADA for R (Helsel 2013). Without the availability of this option, the user has to compute decision and test statistics for one variable at a time which becomes cumbersome when dealing with a large number of variables. ProUCL 5.0 also has the capability of processing data by groups. ProUCL 5.0 is easy to use; it does not require any programming skills as needed when using programs written in R Script.

Deficiencies Identified in ProUCL 5.0: For ProUCL to be compatible with Microsoft Office 8 and provide Excel-compatible Spreadsheet functionality (e.g., ability to input/output *.xlsx files), ProUCL 5.0 used FarPoint Spread 5 for .NET; and for graphics, ProUCL 5.0 used the development software package, ChartFx 7. The look and feel of ProUCL 5.0 is quite different from its previous versions; all main menu options were re-arranged. However, the use of upgraded development softwares resulted in some problems. Specifically, it takes an unacceptably long time to save large ProUCL 5.0 generated output files using FarPoint Spread 5. Also the use of ChartFx 7 caused some problems in properly labeling axes for histograms. Additionally some unhandled exceptions and crashes were noted by users. The unhandled exceptions were mainly noted for "bad" data sets including data sets not following ProUCL input format; data sets with not enough observations; and data sets with not enough detects.

ProUCL 5.1: ProUCL 5.1 represents an upgrade of ProUCL 5.0 to address deficiencies identified in ProUCL 5.0. ProUCL 5.1 retains all capabilities of ProUCL 5.0 as described above. All modules in ProUCL 5.1, and their look and feel is the same as in ProUCL 5.0. In this document, any statement made about the capabilities of ProUCL 5.0 also apply to ProUCL version 5.1; and to save time, not all screen shots used in ProUCL 5.0 manuals have been replaced in the ProUCL 5.1 User Guide and Technical Guide. Upgrades in ProUCL 5.1 (not available in earlier versions) have been labeled as New in ProUCL 5.1 in this document.

All known bugs, crashes, and unhandled exceptions (e.g., on bad data sets) found in ProUCL 5.0 have been addressed in ProUCL 5.1. In ProUCL 5.1, some enhancements have been made in the **Trend Analysis** option of the **Statistical Test** module of ProUCL 5.1. ProUCL 5.1 computes and outputs residuals for the non-parametric T-S trend line which may be helpful to compute a prediction band around the T-S trend line. In addition to generating Q-Q plots based upon detected observations, the **Goodness of Fit Tests** option of the **Statistical Tests** module of ProUCL 5.1 generates censored probability plots for data sets with NDs. Some changes have been made in the decision table used to make suggestions for UCL selection based upon a gamma distribution. New licensing agreements were obtained for the development softwares: FarPoint and ChartFx. Due to deficiencies present in the development software, ProUCL 5.1 generated large output files still take a long time to be saved. However, there is a quick work around to this problem, instead of saving the output sheet using ProUCL, one can copy the output spreadsheet and save the copied output sheet using Excel. This operation can be carried out instantly. Also, ChartFx 7.0 has some deficiencies, and labeling along the x-axis on a histogram is still not as desirable as one would like it to be. Some tools have been added in ProUCL 5.1, and relevant statistics (e.g., start point, midpoint, and end point) of a histogram bar can be displayed by hovering the cursor on that bar.

Software ProUCL version 5.1, its earlier versions: ProUCL version 3.00.02, 4.00.02, 4.00.04, 4.1.00, 4.1.01 and ProUCL 5.0, associated Facts Sheet, User Guides and Technical Guides (e.g., EPA [2004, 2007, 2009a, 2009b, 2010a, 2010b, 2013a, 2013b]) can be downloaded from the EPA website:

http://www.epa.gov/osp/hstl/tsc/software.htm
http://www.epa.gov/osp/hstl/tsc/softwaredocs.htm

The Need for ProUCL Software

EPA guidance documents (e.g., EPA [1989a, 1989b, 1992a, 1992b, 1994, 1996, 2000, 2002a, 2002b, 2002c, 2006a, 2006b, 2009a, and 2009b]) describe statistical methods including: DQOs-based sample size determination procedures, methods to compute decision statistics: UCL95, UPL, and UTLs, parametric and nonparametric hypotheses testing approaches, Oneway ANOVA, OLS regression, and trend determination approaches. Specifically, EPA guidance documents (2000, 2002c, 2006a, 2006b) describe DQOs-based parametric and nonparametric minimum sample size determination procedures needed: to compute decision statistics (e.g., UCL95); to perform site versus background comparisons (e.g., t-test, proportion test, WMW test); and to determine the number of discrete items (e.g., drums filled with hazardous material) that need to be sampled to meet the DQOs (e.g., specified proportion, p_0 of defective items, allowable error margin in an estimate of mean). Statistical methods are used to compute test statistics (e.g., S-W test, t-test, WMW test, T-S trend statistic) and decision statistics (e.g., 95% UCL, 95% UPL, UTL95-95) needed to address statistical issues associated with CERCLA and RCRA site projects. For example, exposure and risk management and cleanup decisions in support of EPA projects are often made based upon the mean concentrations of the contaminants/constituents of potential concern (COPCs). Site-specific BTVs are used in site versus background evaluation studies. A UCL95 is used to estimate the EPC terms (EPA 1992a, 2002a); and upper limits such as upper percentiles, UPLs, or UTLs are used to estimate BTVs or not-to-exceed values (EPA 1992b, 2002b, and 2009). The estimated BTVs are used to address several objectives: to identify the COPCs; to identify the site areas of concern (AOCs); to perform intra-well comparisons to identify MWs not meeting specified standards; and to compare onsite constituent concentrations with site-specific background level constituent concentrations. Oneway ANOVA is used to perform inter-well comparisons and OLS regression and trend tests are often used to determine potential trends present in constituent concentrations identified in GW monitoring wells (MWs). Most of the methods described in this paragraph are available in the ProUCL 5.1 (ProUCL 5.0) software package.

It is noted that not much guidance is available in the guidance documents cited above to compute rigorous UCLs, UPLs, and UTLs for moderately to highly skewed uncensored and left-censored data sets containing NDs with multiple DLs, a common occurrence in environmental data sets. Several parametric and nonparametric methods are available in the statistical literature (Singh, Singh, and Engelhardt 1997; Singh, Singh, and Iaci 2002; Krishnamoorthy *et al*. 2008; Singh, Maichle, and Lee, 2006) to compute UCLs and other upper limits which adjust for data skewness. During the years, as new methods became available to address statistical issues related to environmental projects, those methods were incorporated in ProUCL software so that environmental scientists and decision makers can make more accurate and informed decisions. Until 2006, not much guidance was provided on how to compute UCL95s of the mean and other upper limits (e.g., UPLs and UTLs) based upon data sets containing NDs with multiple DLs. For data sets with NDs, Singh, Maichle, and Lee (2006) conducted an extensive simulation study to compare the performances of the various estimation methods (in terms of bias in the mean estimate) and UCL computation methods (in terms of coverage provided by a UCL). They demonstrated that the nonparametric KM method performs well in terms of bias in estimates of mean. They also concluded that UCLs computed using the Student's t-statistic and percentile bootstrap method using the KM estimates do not provide the desired coverage to the population mean of skewed data sets. They demonstrated that depending upon sample size and data skewness, UCLs computed using KM estimates, the BCA bootstrap method (mildly skewed data sets), the bootstrap-t method, and the Chebyshev inequality (moderately to highly skewed data sets) provide better coverage (closer to the specified 95% coverage) to the population mean than other UCL computation methods. Based upon their findings, during 2006-2007, several UCL and other upper limits computation methods based upon KM and ROS estimates were incorporated in the ProUCL 4.0 software. It is noted that since the inclusion of the KM method in ProUCL 4.0 (2007), the use of the KM method based upper limits has become popular in many environmental applications to estimate EPC terms and BTVs. The KM method is also described in the latest version of the unified RCRA guidance document (U.S. EPA 2009).

It is not easy to justify distributional assumptions of data sets consisting of both detects and NDs with multiple DLs. Therefore, based upon the published literature and experience, parametric UCL (and other upper limits) computation methods such as the MLE method (Cohen 1991) and the expectation maximization (EM) method (Gleit 1985) for normal and lognormal distributions were not included ProUCL 5.0 (and ProUCL 5.1) even though these methods were available in earlier versions of ProUCL. Additionally, the winsorization method (Gilbert 1987) available in an earlier version of ProUCL has also been excluded from ProUCL 5.0 (ProUCL 5.1) due to its poor performance. During 2015, some researchers (e.g., from New Mexico State University, Las Cruces, NM) suggested that the EM method performs better than some of the methods available in ProUCL 5.0, especially the gamma ROS (GROS) method; a method which can be used on left-censored data sets with multiple DLs. The literature has articles dealing with MLE and EM methods for data sets with a single censoring point (DL). Further research needs to be conducted on methods for computing reliable estimates of the mean, *sd*, and upper limits based upon parametric MLE and EM methods for data sets with NDs and multiple DLs. As always, it is the desire of the developers of ProUCL to incorporate the best available methods in ProUCL. The developers of ProUCL welcome/encourage other researchers to share their findings about the EM method showing that EM method performs better than methods already available in ProUCL 5.0/ProUCL 5.1 for data sets with single/multiple censoring points. The developers of ProUCL have been enhancing the ProUCL software with better performing methods as those methods become available. Efforts will be made to incorporate contributed code (with acknowledgement) for superior methods in future versions of ProUCL. ProUCL software is also used for teaching environmental statistics courses therefore, in addition to statistical and graphical methods routinely used to address statistical needs of environmental projects, some poor performing methods such as the substitution DL/2 method and Land's (1975) H-statistic based UCL computation method have been retained in ProUCL version 5.1 for research and comparison purposes.

Methods incorporated in ProUCL 5.1 and in its earlier versions have been tested and verified extensively by the developers, researchers, scientists, and users. Specifically, the results obtained by ProUCL 5.1 are in agreement with the results obtained by using other software packages including Minitab, SAS®, and programs available in R-Script (not all methods are available in these software packages). Additionally, like ProUCL 5.0, ProUCL 5.1 outputs several intermediate results (e.g., khat and biased corrected kstar estimates of the gamma shape parameter, *k*, and critical values (e.g., tolerance factor, K, used to compute UTLs; critical value, d2max, used to compute USL) needed to compute decision statistics of interest, which may help interested users to verify statistical results computed by the ProUCL software. Whenever applicable, ProUCL provides warning messages and based upon professional experience and findings of simulation studies, makes suggestions to help a typical user in selecting the most appropriate decision statistic (e.g., UCL).

Note: The availability of intermediate results and critical values can be used to compute lower limits and two-sided intervals which are not as yet available in the ProUCL software.

For left-censored data sets, ProUCL 5.1 computes decision statistics (e.g., UCL, UPL, and UTL) based upon KM estimates computed in a straight forward manner without flipping the data and re-flipping the decision statistics; these operations are not easy for a typical user to understand and perform and can become quite tedious when multiple analytes need to be processed. Moreover, in environmental applications it is important to compute accurate estimates of *sd* which are needed to compute decision making statistics including UPLs and UTLs. Decision statistics (UPL, UTL) based upon a KM estimate of the of *sd* and computed using indirect methods can be different from the statistics computed using an estimate of *sd* obtained using the KM method directly, especially when one is dealing with a skewed data set or when using a log-transformation. These issues are elaborated by examples discussed in the accompanying ProUCL 5.1 Technical Guide.

For uncensored data sets, researchers (e.g., Johnson 1978; Chen 1995; Efron and Tibshirani 1993; Hall [1988, 1992], and additional references found in Chapters 2 and 3) developed parametric (e.g., gamma distribution based) and nonparametric (bootstrap-t and Hall's bootstrap method, modified-t) methods for computation of decision statistics which adjust for data skewness. For uncensored positively skewed data sets, Singh, Singh, and Iaci (2002) and Singh and Singh (2003) performed simulation experiments to compare the performances (in terms of coverage probabilities) of the various UCL computation methods described in the literature. They demonstrated that for skewed data sets, UCLs based upon Student's t statistic, central limit theorem (CLT), and percentile bootstrap method tend to underestimate the population mean (EPC). It is reasonable to state that the findings of the simulation studies performed on uncensored skewed data sets comparing the performances of the various UCL computation methods can be extended to skewed left-censored data sets. Based upon the findings of those studies performed on uncensored data sets and also using the findings summarized in Singh, Maichle, and Lee (2006), it was concluded that t-statistic, CLT, and the percentile bootstrap method based UCLs computed using KM estimates (and also ROS estimates) underestimate the population mean of moderately skewed to highly skewed data sets. Interested users may want to verify these statements by performing simulation experiments or other forms of rigorous testing. Like uncensored skewed data sets, for left-censored data sets, ProUCL 5.1 offers several parametric and nonparametric methods for computing UCLs and other limits which adjust for data skewness.

Due to the lack of research and methods, in earlier versions of the ProUCL software (e.g., ProUCL 4.00.02, ProUCL 4.0), KM estimates were used in the normal distribution based equations for computing the various upper limits for left-censored data sets. However, normal distribution based upper limits (e.g., t-UCL) using KM estimates (or any other estimates such as ROS estimates) fail to provide the specified coverage (e.g., 0.95) of the parameters (e.g., mean, percentiles) of populations with skewed distributions (Singh, Singh, Iaci 2002; Johnson 1978; Chen 1995). For skewed data sets, ProUCL 5.0/ProUCL 5.1 computes UCLs applying KM estimates in UCL equations for skewed data sets (e.g., gamma and lognormal); therefore, some changes have been made in the decision tables of ProUCL 5.0/ProUCL 5.1 for computing UCL95s. Also, the nonparametric UCL computation methods (e.g., percentile bootstrap) do not provide the desired coverage to the population means of skewed distributions (e.g., Hall [1988, 1992], Efron and Tibshirani, 1993). For example, the use of t-UCL or the percentile bootstrap UCL method on robust ROS estimates or on KM estimates underestimates the population mean for moderately skewed to highly skewed data sets. Chapters 3 and 5 of the ProUCL Technical Guide describe parametric and nonparametric KM methods for computing upper limits (and available in ProUCL 5.0/ ProUCL 5.1) which adjust for data skewness.

The KM method yields good estimates of the population mean and *std* (Singh, Maichle, and Lee 2006); however upper limits computed using the KM or ROS estimates in normal equations or in the percentile bootstrap method do not account for skewness present in the data set. Appropriate UCL computation methods which account for data skewness should be used on KM or ROS estimates. For left-censored data sets, ProUCL 5.0/ProUCL 5.1 compute upper limits using KM estimates in gamma (lognormal) UCL, UPL, and UTL equations (e.g., also suggested in U.S. EPA 2009) provided the detected observations in the left-censored data set follow a gamma (lognormal) distribution.

Recently, the use of the ISM methodology has been recommended (ITRC 2012) for collecting soil samples with the purpose of estimating mean concentrations of DUs requiring analysis of human and ecological risk and exposure. ProUCL can be used to compute UCLs based upon ISM data as described and recommended in the ITRC ISM Technical and Regulatory Guide (2012). At many sites, large amounts of discrete background data are already available which are not directly comparable to the actual field ISM data (onsite or background). To compare the existing discrete background data with field ISM data, the **BISS** module (blocked for general use in ProUCL version 5.1 awaiting guidance and instructions for its intended use) of ProUCL 5.1 can be used on a large (e.g., consisting of at least 30 observations) existing discrete background data set. The **BISS** module simulates the incremental sampling methodology based equivalent incremental background samples; and each simulated BISS sample represents an estimate of the mean of the population represented by the discrete background data set. The availability of a large discrete background data set collected from areas with geological conditions comparable to the DU(s) of interest (onsite DUs) is a requirement for successful application of this module. The user cannot see the simulated BISS data; however, the simulated BISS data can be accessed by other modules of ProUCL 5.0 (ProUCL 5.1) for performing desired statistical evaluations. For example, the simulated BISS data can be merged with the actual field ISM background data after comparing the two data sets using a two-sample t-test. The actual field ISM or the merged ISM and BISS data can be accessed by modules of ProUCL to compute a UCL of the mean or a UTL.

ProUCL 5.1 Capabilities

Assumptions: Like most statistical methods, statistical methods for computing upper limits (e.g., UCLs, UPLs, UTLs) are also based upon certain assumptions including the availability of a randomly collected data set consisting of independently and identically distributed (*i.i.d*) observations representing the population (e.g., site area, reference area) under investigation. A UCL of the mean (of a population) and BTV estimates (UPL, UTL) should be computed using a randomly collected (simple random or systematic random) data set representing a single statistical population (e.g., site population or background population). When multiple populations (e.g., background and site data mixed together) are present in a data set, the recommendation is to separate them first by using the population partitioning techniques (e.g., Singh, Singh, and Flatman 1994) prior to computing the appropriate decision statistics (e.g., 95% UCLs). Regardless of how the populations are separated, decision statistics should be computed separately for each identified population. The topic of population partitioning and the extraction of a valid site-specific background data set from a broader mixture data set potentially consisting of both onsite and offsite data are beyond the scope of ProUCL 5.0/ProUCL 5.1. Parametric estimation and hypotheses testing methods (e.g., t-test, UCLs, UTLs) are based upon distributional (e.g., normal distribution, gamma) assumptions. ProUCL includes GOF tests for determining if a data set follows a normal, a gamma, or a lognormal distribution.

Multiple Constituents/Variables: Environmental scientists need to evaluate many constituents in their decision making processes including exposure and risk assessment, background evaluations, and site versus background comparisons. ProUCL can process multiple constituents/variables simultaneously in a user-friendly manner; an option not available in other freeware or commercial software packages such as NADA for R (Helsel 2013). This option is very useful when one has to process many variables/analytes and compute decision statistics (e.g., UCLs, UPLs, and UTLs) and/or test statistics (e.g., ANOVA test, trend test) for those variables/analytes.

Analysis by a Group Variable: ProUCL also has the capability of processing data by groups. A valid group column should be included in the data file. The analyses of data categorized by a group ID variable such as: 1) Surface versus (vs.) Subsurface; 2) AOC1 vs. AOC2; 3) Site vs. Background; and 4) Upgradient vs. Downgradient MWs are common in many environmental applications. ProUCL offers this option for data sets with and without nondetects. The **Group** option provides a way to perform statistical tests and methods including graphical displays separately for each of the group (samples from different populations) that may be present in a data set. For example, the same data set may consist of analytical data from multiple groups or populations representing site, background, two or more AOCs, surface soil, subsurface soil, and GW. By using this option, the graphical displays (e.g., box plots, Q-Q plots, histograms) and statistics (including computation of background statistics, UCLs, ANOVA test, trend test and OLS regression statistics) can be easily computed separately for each group in the data set.

<u>Exploratory Graphical Displays for Uncensored and Left-Censored Data Sets:</u> Graphical methods included in the **Graphs** module of ProUCL include: Q-Q plots (data in same column), multiple Q-Q plots (data in different columns), box plots, multiple box plots (data in different columns), and histograms. These graphs can also be generated for data sets containing ND observations. Additionally, the **OLS Regression** and **Trend Analysis** module can be used to generate graphs displaying parametric OLS regression lines with confidence and prediction intervals around the regression and nonparametric Theil-Sen trend lines. The **Trend Analysis** module can generate trend graphs for data sets without a sampling event variable, and also generates time series graphs for data sets with a sampling event (time) variable. Like ProUCL 5.0, ProUCL 5.1 accepts only numerical values for the event variable. Graphical displays of a data set are useful for gaining added insight regarding a data set that may not otherwise be clear by looking at test statistics such as T-S test or MK statistics. Unlike test statistics (e.g., t-test, MK test, AD test) and decision statistics (e.g., UCL, UTL), graphical displays do not get influenced by outliers and ND observations. It is suggested that the final decisions be made based upon statistical results as well as graphical displays.

Side-by-side box plots or multiple Q-Q plots are useful to graphically compare concentrations of two or more groups (e.g., several monitoring wells). The GOF module of ProUCL generates Q-Q plots for normal, gamma, and lognormal distributions based upon uncensored as well as left-censored data sets with NDs. All relevant information such as the test statistics, critical values and probability-values (*p*-values), when available are also displayed on the GOF Q-Q plots. In addition to providing information about the data distribution, a normal Q-Q plot in the original raw scale also helps to identify outliers and multiple populations that may be present in a data set. On a Q-Q plot, observations well-separated from the majority of the data may represent potential outliers coming from a population different from the main dominant population (e.g., background population). In a Q-Q plot, jumps and breaks of significant magnitude suggest the presence of observations coming from multiple populations (onsite and offsite areas). ProUCL can also be used to display box plots with horizontal lines displayed/superimposed at pre-specified compliance limits (CLs) or computed upper limits (e.g., UPL, UTL). This kind of graph provides a visual comparison of site data with compliance limits and/or BTV estimates.

<u>Outlier Tests:</u> ProUCL also provides a couple of classical outlier test procedures (EPA 2006b, 2009), the Dixon test and the Rosner test. The details of these outlier tests are described in Chapter 7. These outlier tests often suffer from “masking effects” in the presence of multiple outliers. It is suggested that the classical outlier procedures should always be accompanied by graphical displays including box plots and Q-Q plots. Description and use of the robust and masking-resistant outlier procedures (Rousseeuw and Leroy 1987; Singh and Nocerino 1995) are beyond the scope of ProUCL 5.1. Interested users are encouraged to try the Scout 2008 software package (EPA 2009d) for robust outlier identification methods especially when dealing with multivariate data sets consisting of observations for several variables/analytes/constituents.

Outliers represent observations coming from populations different from the main dominant population represented by the majority of the data set. Outliers distort most statistics (e.g., mean, UCLs, UPLs, test statistics) of interest. Therefore, it is desirable to compute decisions statistics based upon data sets representing the main population and not to compute distorted statistics by accommodating a few low probability outliers (e.g., by using a lognormal distribution). Moreover, it should be noted that even though outliers might have minimal influence on hypotheses testing statistics based upon ranks (e.g., WMW test), outliers do distort several nonparametric statistics including bootstrap methods such as bootstrap-t and Hall's bootstrap UCLs and other nonparametric UPLs and UTLs computed using higher order statistics.

Goodness-of-Fit Tests: In addition to computing simple summary statistics for data sets with and without NDs, ProUCL 5.1 includes GOF tests for normal, lognormal and gamma distributions. To test for normality (lognormality) of a data set, ProUCL includes the Lilliefors test and the extended S-W test for samples of sizes up to 2000 (Royston 1982, 1982a). For the gamma distribution, two GOF tests: the A-D test (Anderson and Darling 1954) and K-S test (Schneider 1978) are available in ProUCL. For samples of larger sizes (e.g., with $n > 100$) and small values of the gamma shape parameter, k (e.g., $k \leq 0.1$), significant discrepancies were found in the critical values of the two gamma GOF test statistics (A-D and K-S tests) obtained using the two gamma deviate generation algorithms: Whitaker (1974) and Marsaglia and Tsang (2000). In ProUCL 5.0 (and ProUCL 5.1), for values of $k \leq 0.2$, the critical values of the two gamma GOF tests: A-D and K-S tests have been updated using the currently available more efficient gamma deviate generation algorithm due to Marsaglia and Tsang's (2000); more details about the implementation of their algorithm can be found in Kroese, Taimre, and Botev (2011). For these two GOF and values of the shape parameter, $k=0.025, 0.05, 0.1$, and 0.2, critical value tables have been updated by incorporating the newly generated critical values for three levels of significance: 0.05, 0.1, and 0.01. The updated tables are provided in Appendix A of the ProUCL Technical Guide. It was noted that for $k=0.2$, the older (generated in 2002) and the newly generated critical values are in general agreement; therefore, critical values for $k=0.2$ were not replaced in tables summarized in Appendix A.

ProUCL also generates GOF Q-Q plots for normal, lognormal, and gamma distributions displaying all relevant statistics including GOF test statistics. GOF tests for data sets with and without NDs are described in Chapters 2 and 3 of the ProUCL Technical Guide. For data sets containing NDs, it is not easy to verify the distributional assumptions correctly, especially when the data set consists of a large percentage of NDs with multiple DLs and NDs exceeding some detected values. Historically, decisions about distributions of data sets with NDs are based upon GOF test statistics computed using the data obtained: without NDs; replacing NDs by 0, DL, or DL/2; using imputed NDs based upon a ROS (e.g., lognormal ROS) method. For data sets with NDs, ProUCL 5.1 can perform GOF tests using the methods listed above. ProUCL 5.1 can also generate censored probability plots (Q-Q plots) which are very similar to Q-Q plots generated using detected data. Using the **Imputed NDs using ROS Methods** option of the **Stats/Sample Sizes** module of ProUCL 5.0, additional columns can be generated for storing imputed (estimated) values for NDs based upon normal ROS, gamma ROS, and lognormal ROS (also known as robust ROS) methods.

Sample Size Determination and Power Evaluation: The **Sample Sizes** module in ProUCL can be used to develop DQO-based sampling designs needed to address statistical issues associated with environmental projects. ProUCL 5.1 provides user-friendly options for entering the desired/pre-specified values for decision parameters (e.g., Type I and Type II error rates) and other DQOs used to determine minimum sample sizes for statistical applications including: estimation of the mean, single and two-sample hypothesis testing approaches, and acceptance sampling for discrete items (e.g., drums containing hazardous waste). Both parametric (e.g., t-test) and nonparametric (e.g., Sign test, WRS test) sample size determination methods as described in EPA (2000, 2002c, 2006a, 2006b) guidance documents are available in ProUCL 5.1. ProUCL also has the sample size determination option for acceptance sampling of lots of discrete objects such as a lot (batch, set) of drums containing hazardous waste (e.g., RCRA applications, EPA 2002c). When the sample size for an application (e.g., verification of cleanup level) is not computed using the DQOs-based sampling design process, the **Sample Size** module can be used to assess the power of the test statistic used in retrospect. The mathematical details of the **Sample Sizes** module are given in Chapter 8 of the ProUCL Technical Guide.

Bootstrap Methods: Bootstrap methods are computer intensive nonparametric methods which can be used to compute decision statistics of interest when a data set does not follow a known distribution, or when it is difficult to analytically derive the distributions of statistics of interest. It is well-known that for moderately skewed to highly skewed data sets, UCLs based upon standard bootstrap and the percentile bootstrap methods do not perform well (e.g., Efron [1981, 1982]; Efron and Tibshirani 1993; Hall [1988,1992]; Singh, Singh, and Iaci 2002; Singh and Singh 2003, Singh, Maichle and Lee 2006) as the interval estimates based upon these bootstrap methods fail to provide the specified coverage to the population mean (e.g., UCL95 does not provide adequate 95% coverage of population mean). For skewed data sets, Efron and Tibshirani (1993) and Hall (1988, 1992) considered other bootstrap methods such as the BCA, bootstrap-t and Hall's bootstrap methods. For skewed data sets, bootstrap-t and Hall's bootstrap (meant to adjust for skewness) methods perform better (e.g., in terms of coverage for the population mean) than the other bootstrap methods. However, it has been noted (e.g., Efron and Tibshirani 1993, Singh, Singh, and Iaci 2002) that these two bootstrap methods tend to yield erratic and inflated UCL values (orders of magnitude higher than other UCLs) in the presence of outliers. Similar behavior of the bootstrap-t UCL and Hall's bootstrap UCL methods is observed for data sets consisting of NDs and outliers. For nonparametric uncensored and left-censored data sets with NDs, depending upon data variability and skewness, ProUCL recommends the use of BCA bootstrap, bootstrap-t, or Chebyshev inequality based methods for computing decision statistics. Due to the reasons described above, whenever applicable, ProUCL 5.0/ProUCL 5.1 provides cautionary notes and warning messages regarding the use of bootstrap-t and Halls bootstrap UCL methods.

Hypotheses Testing Approaches: ProUCL software has both single-sample (e.g., Student's t-test, sign test, proportion test, WSR test) and two-sample (Student's t-test, WMW test, Gehan test, and T-W test) parametric and nonparametric hypotheses testing approaches. Hypotheses testing approaches in ProUCL can handle both full-uncensored data sets and left-censored data sets with NDs. Most of the hypotheses tests also report associated *p*-values. For some hypotheses tests (e.g., WMW test, WSR test, proportion test), large sample *p*-values based upon the normal approximation are computed using continuity correction factors. The mathematical details of the various single-sample and two-sample hypotheses testing approaches are described in Chapter 6 the ProUCL Technical Guide.

- Single-Sample Tests: Parametric (Student's t-test) and nonparametric (Sign test, WSR test, tests for proportions and percentiles) hypotheses testing approaches are available in ProUCL. Single-sample hypotheses tests are used when environmental parameters such as the cleanup standard, action level, or compliance limits are known, and the objective is to compare site concentrations with those known threshold values. A t-test (or a sign test) may be used to verify the attainment of cleanup levels in an AOC after a remediation activity has taken place or a test for proportion may be used to verify if the proportion of exceedances of an action level (A_0 or a CL) by sample observations collected from an AOC (or a MW) exceeds a certain specified proportion (e.g., 1%, 5%, 10%).

  The differences between these tests should be noted and understood. A t-test or a Wilcoxon Signed Rank (WSR) test are used to compare the measures of location and central tendencies (e.g., mean, median) of a site area (e.g., AOC) to a cleanup standard, C_s, or action level also representing a measure of central tendency (e.g., mean, median); whereas, a proportion test determines if the proportion of site observations from an AOC exceeding a compliance limit (CL) exceeds a specified proportion, P_0 (e.g., 5%, 10%). The percentile test compares a specified percentile (e.g., 95^{th}) of the site data to a pre-specified upper threshold (e.g., action level).

- Two-Sample Tests: Hypotheses tests (Student's t-test, WMW test, Gehan test, T-W test) are used to perform site versus background comparisons, compare concentrations of two or more AOCs, or to compare concentrations of GW collected from MWs. As cited in the literature, some of the hypotheses testing approaches (e.g., nonparametric two-sample WMW) deal with a single detection limit scenario. When using the WMW test on a data set with multiple detection limits, all observations (detects and NDs) below the largest detection limit need to be considered as NDs (Gilbert 1987). This in turn tends to reduce the power and increase uncertainty associated with test. As mentioned before, it is always desirable to supplement the test statistics and conclusions with graphical displays such as multiple Q-Q plots and side-by-side box plots. The Gehan test or T-We (new in ProUCL 5.1) should be used in cases where multiple detection limits are present.

Note about Quantile Test: For smaller data sets, the Quantile test as described in U.S. EPA documents (U.S. EPA [1994, 2006b]; Hollander and Wolfe, 1999) is available in ProUCL 4.1(see ProUCL 4.1 Technical Guide). In the past, some users incorrectly used this test for larger data sets. Due to lack of resources, this test has not been expanded for data sets of all sizes. Therefore, to avoid confusion and its misuse for larger data sets, the Quantile test was not included in ProUCL 5.0 and ProUCL 5.1.

Computation of Upper Limits including UCLs, UPLs, UTLs, and USLs: ProUCL software has parametric and nonparametric methods including bootstrap and Chebyshev inequality based methods to compute decision making statistics such as UCLs of the mean (EPA 2002a), percentiles, UPLs for future k ($\geq$1) observations, UTLs (U.S. EPA [1992b and 2009]) and upper simultaneous limits (USLs) (Singh and Nocerino [1995, 2002]) based upon uncensored full data sets and left-censored data sets containing NDs with multiple DLs. Methods incorporated in ProUCL cover a wide range of skewed data distributions with and without NDs. In addition to normal and lognormal distributions based upper limits, ProUCL 5.0 can compute parametric UCLs, percentiles, UPLs for future k ($\geq$1) observations, UTLs, and USLs based upon gamma distributed data sets. For data sets with NDs, ProUCL has several estimation methods including the Kaplan-Meier (KM) method (1958), ROS methods (Helsel 2005) and substitution methods such as replacing NDs with the DL or DL/2 (Gilbert 1987; U.S. EPA 2006b). Substitution method and other poor performing methods (e.g., H-UCL for lognormal distribution) have been retained, as requested by U.S. EPA scientists, in ProUCL 5.0/ProUCL 5.1 for research and comparison purposes. *One may not interpret the availability of these poor performing methods in ProUCL as recommended methods by ProUCL or by the U.S EPA for computing decision statistics.*

Computation of UCLs Based upon Uncensored Data Sets without NDs: Parametric UCL computation methods in ProUCL for uncensored data sets include: Student's t-UCL, Approximate gamma UCL (using chi-square approximation), Adjusted gamma UCL (adjusted for level significance), Land's H-UCL, and Chebyshev inequality-based UCL (using minimum variance unbiased estimates (MVUEs) of parameters of a lognormal distribution). Nonparametric UCL computation methods for data sets without NDs include: CLT-based UCL, Modified-t-statistic-based UCL (adjusted for skewness), Adjusted-CLT-based UCL (adjusted for skewness), Chebyshev inequality-based UCL (using sample mean and standard deviation), Jackknife method-based UCL, UCL based upon standard bootstrap, UCL based upon percentile bootstrap, UCL based upon BCA bootstrap, UCL based upon bootstrap-t, and UCL based upon Hall's bootstrap method. The details of UCL computation methods for uncensored data sets are summarized in Chapter 2 of the ProUCL Technical Guide.

Computations of UPLs, UTLs, and USLs Based upon Uncensored Data Sets without NDs: For uncensored data sets without NDs, ProUCL can compute parametric percentiles, UPLs for k (k≥1) future observations, UPLs for mean of k (≥1) future observations, UTLs, and USLs based upon the normal, gamma, and lognormal distributions. Nonparametric upper limits are typically based upon order statistics of a data set. Depending upon the size of the data set, the higher order statistics (maximum, second largest, third largest, and so on) are used to compute these upper limits (e.g., UTLs). Depending upon the sample size, specified CC and coverage probability, ProUCL 5.1 outputs the actual CC achieved by a nonparametric UTL. The details of the parametric and nonparametric computation methods for UPLs, UTLs, and USLs are described in Chapter 3 of the ProUCL Technical Guide.

Computation of UCLs, UPLs, UTLs, and USLs Based upon Left-Censored Data Sets with NDs: For data sets with NDs, ProUCL computes UCLs, UPLs, UTLs, and USLs based upon the mean and *sd* computed using lognormal ROS (LROS, robust ROS), Gamma ROS (GROS), KM, and DL/2 substitution methods. To adjust for skewness in non-normally distributed data sets, ProUCL uses bootstrap methods and Chebyshev inequality when computing UCLs and other limits using estimates of the mean and *sd* obtained using the methods (details in Chapters 4 and 5) listed above. ProUCL 5.1 (new in ProUCL 5.0) uses parametric methods on KM (and ROS) estimates, provided detected observations in the left-censored data set follow a parametric distribution. For example, if the detected data follow a gamma distribution, ProUCL uses KM estimates in gamma distribution-based equations when computing UCLs, UTLs, and other upper limits. When detected data do not follow a discernible distribution, depending upon size and skewness of detected data, ProUCL recommends the use of Kaplan-Meier (1958) estimates in bootstrap methods and the Chebyshev inequality for computing nonparametric decision statistics (e.g., UCL95, UPL, UTL) of interest. ProUCL computes KM estimates directly using left-censored data sets without flipping data and requiring re-flipping of decision statistics. The KM method incorporated in ProUCL computes both *sd* and standard error (*SE*) of the mean. As mentioned earlier, for historical reasons and for comparison and research purposes, the DL/2 substitution method and H-UCL based upon LROS method have been retained in ProUCL 5.0/ProUCL 5.1. The inclusion of the substitution and LROS methods in ProUCL should not be inferred as an endorsement of those methods by ProUCL software and its developers. The details of the UCL computation methods for data sets with NDs are given in Chapter 4 and the detail description of the various other upper limits: UPLs, UTLs, and USLs for data sets with NDs are given in Chapter 5 of the ProUCL Technical Guide.

Oneway ANOVA, OLS Regression and Trend Analysis: The **Oneway ANOVA** module has both classical and nonparametric K-W ANOVA tests as described in EPA guidance documents (e.g., EPA [2006b, 2009]). Oneway ANOVA is used to compare means (or medians) of multiple groups such as comparing mean concentrations of several areas of concern or performing inter-well comparisons of COPC concentrations at several MWs. The **OLS Regression** option computes the classical OLS regression line and generates graphs displaying the OLS line, confidence bands and prediction bands around the regression line. All statistics of interest including slope, intercept, and correlation coefficient are displayed on the OLS line graph. The **Trend Analysis** module has two nonparametric trend tests: the M-K trend test and T-S trend test. Using this option, one can generate trend graphs and time-series graphs displaying a T-S trend line and all other statistics of interest with associated *p*-values. In addition to slope and intercept, the T-S test in ProUCL 5.1 computes and outputs residuals based upon the computed nonparametric T-S line.

In GW monitoring applications, OLS regression, trend tests, and time series plots are often used to identify trends (e.g., upwards, downwards) in constituent concentrations of GW monitoring wells over a certain period of time (U.S. EPA 2009). The details of Oneway ANOVA are given in Chapter 9 and OLS regression line and Trend tests methods are described in Chapter 10 of the ProUCL Technical Guide.

BISS Module: At many sites, a large amount of discrete onsite and background data are already available which are not directly comparable to actual field ISM data. In order to provide a tool to compare the existing discrete data with ISM data, the **BISS** module of ProUCL 5.0 may be used on a large existing discrete data set. The ISM methodology used to develop the **BISS** module is a relatively new approach; methods incorporated in this BISS module require further investigation. For now, the **BISS** module has been blocked for use in ProUCL 5.0/ProUCL 5.1 as this module is awaiting adequate guidance for its intended use on discrete background data sets.

Recommendations and Suggestions in ProUCL: Until 2006, not much guidance was available on how to compute a UCL95 of the mean and other upper limits (e.g., UPLs and UTLs) for skewed left-censored data sets containing NDs with multiple DLs, a common occurrence in environmental data sets. For uncensored positively skewed data sets, Singh, Singh, and Iaci (2002) and Singh and Singh (2003) performed extensive simulation experiments to compare the performances (in terms of coverage probabilities) of several UCL computation methods described in the statistical and environmental literature. They noted that the optimal choice of a decision statistic (e.g., UCL95) depends upon the sample size, data distribution and data skewness. They incorporated the results of their findings in ProUCL 3.1 and higher versions to select the most appropriate UCL to estimate the EPC term.

For data sets with NDs, Singh, Maichle, and Lee (2006) conducted a similar simulation study to compare the performances of the various estimation methods (in terms of bias in the mean estimate); and some UCL computation methods (in terms of coverage provided by a UCL). They demonstrated that the KM estimation method performs well in terms of bias in estimates of the mean; and for skewed data sets, the t-statistic, CLT, and the percentile bootstrap method based UCLs computed using KM estimates (and ROS estimates) underestimate the population mean. From these findings summarized in Singh, Singh, and Iaci (2002) and Singh, Maichle, and Lee (2006), it is natural to state and assume the findings of the simulation studies performed on uncensored skewed data sets comparing performances of the various UCL computation methods can be extended to skewed left-censored data sets.

Like uncensored data sets without NDs, for data sets with NDs, there is no one single best UCL (and other upper limits such as UTL, UPL) which can be used to estimate an EPC (and background threshold values) for all data sets of varying sizes, distribution, and skewness. The optimal choice of a decision statistic depends upon the size, distribution, and skewness of detected observations.

For data sets with and without NDs, ProUCL computes decision statistics including UCLs, UPLs, and UTLs using several parametric and nonparametric methods covering a wide-range of sample size, data variability and skewness. Using the results and findings summarized in the literature cited above, and based upon the sample size, data distribution, and data skewness, modules of ProUCL make suggestions about using the most appropriate decision statistic(s) to estimate population parameter(s) of interest (e.g., EPC). The suggestions made in ProUCL are based upon the extensive professional applied and theoretical experience of the developers in environmental statistical methods, published literature, results of simulation studies conducted by the developers of ProUCL and procedures described in many U.S. EPA guidance documents. These suggestions are made to help the users in selecting the most appropriate UCL to estimate an EPC which is routinely used in exposure assessment and risk management studies of the U.S. EPA. It should be pointed out that a typical simulation study cannot cover all data sets of various sizes and skewness from all types of distributions. For an analyte (data set) with skewness (*sd* of logged data) near the end points of the skewness intervals described in decision tables of Chapter 2 (e.g., Tables 2-9 through 2-11) of the ProUCL Technical Guide, the user/project team may select the most appropriate UCL based upon the site CSM, expert site knowledge, toxicity of the analyte, and exposure risks associated with that analyte. The project team should make the final decision regarding using or not using the suggestions/recommendations made by ProUCL. If deemed necessary, the project team may want to consult a statistician.

Even though, ProUCL software has been developed using limited government funding, ProUCL 5.1 provides many statistical and graphical methods described in U.S. EPA documents for data sets with and without NDs. However, one may not compare the availability of methods in ProUCL 5.1 with methods available in the commercial software packages such as SAS® and Minitab 16. For example, trend tests correcting for seasonal/spatial variations and geostatistical methods are not available in the ProUCL software. For those methods, the user is referred to commercial software packages such as SAS®. As mentioned earlier, is the developers of ProUCL recommended supplementing test results (e.g., two-sample test) with graphical displays (e.g., Q-Q plots, side-by-side box plots) especially when data sets contain NDs and outliers. With the inclusion of the **BISS**, **Oneway ANOVA**, **OLS Regression Trend** and the user-friendly DQOs based **Sample Size** modules, ProUCL represents a comprehensive software package equipped with statistical methods and graphical tools needed to address many environmental sampling and statistical needs as described in the various CERCLA (U.S. EPA 1989a, 1992a, 2002a, 2002b, 2006a, 2006b), MARSSIM (U.S. EPA 2000), and RCRA (U.S. EPA 1989b, 1992b, 2002c, 2009) guidance documents.

Finally, the users of ProUCL are cautioned about the use of methods and suggestions described in some recent environmental literature. For example, many decision statistics (e.g., UCLs, UPLs, UTLs,) computed using the methods (e.g., percentile bootstrap, statistics using KM estimates and t-critical values) described in Helsel (2005, 2012) will fail to provide the desired coverage for environmental parameters of interest (mean, upper percentile) of moderately skewed to highly skewed populations and conclusions derived based upon those decisions statistics may lead to incorrect conclusions which may not be cost-effective or protective of human health and the environment.

Note about ProUCL 5.1: ProUCL 5.1 represents an upgrade of ProUCL 5.0 to address deficiencies identified in ProUCL 5.0. ProUCL 5.1 retains all capabilities of ProUCL 5.0 as described above. All modules in ProUCL 5.1, and their look and feel is the same as in ProUCL 5.0. In this document, any statement made about the capabilities of ProUCL 5.0 also apply to ProUCL version 5.1; and to save time, not all screen shots used in ProUCL 5.0 manuals have been replaced in the ProUCL 5.1 User Guide and Technical Guide. Upgrades in ProUCL 5.1 (not available in earlier versions) have been labeled as New in ProUCL 5.1 in this document.

ProUCL 5.1 Technical Guide

In addition to this User Guide, a Technical Guide also accompanies the ProUCL 5.1 software, providing details of using the statistical and graphical methods incorporated in ProUCL 5.1. Most of the mathematical algorithms and formulae (with references) used in the development of ProUCL 5.1 are described in the associated Technical Guide.

Chapter 1

Guidance on the Use of Statistical Methods in ProUCL Software

Decisions based upon statistics computed using discrete data sets of small sizes (e.g., < 6) cannot be considered reliable enough to make decisions that affect human health and the environment. For example, a background data set of size < 6 is not large enough to characterize a background population, compute BTV estimates, or to perform background versus site comparisons. Several U.S. EPA guidance documents (e.g., EPA 2000, 2006a, 2006b) detail DQOs and minimum sample size requirements needed to address statistical issues associated with different environmental applications. In order to obtain reliable statistical results, an adequate amount of data should be collected using project-specified DQOs (i.e., CC, decision error rates). The **Sample Sizes** module of ProUCL computes minimum sample sizes based on DQOs specified by the user and described in many guidance documents. In some cases, it may not be possible (e.g., due to resource constraints) to collect the calculated number of samples needed to meet the project-specific DQOs. Under these circumstances one can use the **Sample Sizes** module to assess the power of the test statistic resulting from the reduced number of samples which were collected. Based upon professional experience, the developers of ProUCL 4 software and its later versions have been making some rule-of-thumb suggestions regarding minimum sample size requirements needed to perform statistical evaluations such as: estimation of environmental parameters of interest (i.e., EPCs and BTVs), comparing site data with background data or with some pre-established screening levels (e.g., action levels [ALs], compliance limits [CLs]). Those rule-of thumb suggestions are described later in Section 1.7 of this chapter. It is noted that those minimum sample requirements have been adopted by some other guidance documents including the RCRA Guidance Document (EPA 2009).

This chapter also describes the differences between the various statistical upper limits including upper confidence limits (UCLs) of the mean, upper prediction limits (UPLs) for future observations, and upper tolerance intervals (UTLs) often used to estimate the environmental parameters of interest including EPC terms and BTVs. The use of a statistical method depends upon the environmental parameter(s) being estimated or compared. The measures of central tendency (e.g., means, medians, or their UCLs) are used to compare site mean concentrations with a cleanup standard, C_s, also representing some central tendency measure of a reference area or some other known threshold representing a measure of central tendency. The upper threshold values, such as the CLs, alternative concentration limits (ACL), or not-to-exceed values, are used when individual point-by-point observations are compared with those threshold values. Depending upon whether the environmental parameters (e.g., BTVs, not-to-exceed value, or EPC term) are known or unknown, different statistical methods with different data requirements are needed to compare site concentrations with pre-established (known) or estimated (unknown) standards and BTVs. Several upper limits, and single and two sample hypotheses testing approaches, for both full-uncensored and left-censored data sets are available in the ProUCL software package for performing the comparisons described above.

1.1 Background Data Sets

Based upon the CSM and regional and expert knowledge about the site, the project team selects background or reference areas. Depending upon the site activities and the pollutants, the background area can be site-specific or a general reference area with conditions comparable to the site before contamination due to site related activities. An appropriate random sample of independent observations (*i.i.d*) should be collected from the background area. A defensible background data set represents a "single" environmental population possibly without any outliers. In a background data set, in addition to reporting and/or laboratory errors, statistical outliers may also be present. A few elevated statistical outliers present in a background data set may actually represent potentially contaminated locations belonging to an impacted site area and/or possibly from other sources; those elevated outliers may not be coming from the background population under evaluation. Since the presence of outliers in a data set tends to yield distorted (poor and misleading) values of the decision making statistics (e.g., UCLs, UPLs and UTLs), elevated outliers should not be included in background data sets and estimation of BTVs. The objective here is to compute background statistics based upon a data set which represents the main background population, and does not accommodate the few low probability high outliers (e.g., coming from extreme tails of the data distribution) that may also be present in the sampled data. The occurrence of elevated outliers is common when background samples are collected from various onsite areas (e.g., large Federal Facilities). The proper disposition of outliers, to include or not include them in statistical computations, should be decided by the project team. The project team may want to compute decision statistics with and without the outliers to evaluate the influence of outliers on the decision making statistics.

A couple of classical outlier tests (Dixon and Rosner tests) are available in ProUCL. Since both of these classical tests suffer from masking effects (e.g., some extreme outliers may mask the occurrence of other intermediate outliers), it is suggested that these classical outlier tests be supplemented with graphical displays such as a box plot and a Q-Q plot on a raw scale. The use of exploratory graphical displays helps in determining the number of outliers potentially present in a data set. The use of graphical displays also helps in identifying extreme high outliers as well as intermediate and mild outliers. The use of robust and masking-resistant outlier identification procedures (Singh and Nocerino, 1995, Rousseeuw and Leroy, 1987) is recommended when multiple outliers are present in a data set. Those methods are beyond the scope of ProUCL 5.1. However, several robust outlier identification methods are available in the Scout 2008 version 1.0 software package (EPA 2009d, http://archive.epa.gov/esd/archive-scout/web/html/).

An appropriate background data set of a reasonable size (preferably computed using the DQOs processes) is needed for the data set to be representative of background conditions and to compute upper limits (e.g., estimates of BTVs) and compare site and background data sets using hypotheses testing approaches. A background data set should have a minimum of 10 observations, however more observations is preferable.

1.2 Site Data Sets

A data set collected from a site population (e.g., AOC, exposure area [EA], DU, group of MWs) should be representative of the population under investigation. Depending upon the areas under investigation, different soil depths and soil types may be considered as representing different statistical populations. In such cases, background versus site comparisons may have to be conducted separately for each of those sub-populations (e.g., surface and sub-surface layers of an AOC, clay and sandy site areas). These issues, such as comparing depths and soil types, should also be considered in the planning stages when developing sampling designs. Specifically, the availability of an adequate amount of representative data is required from each of those site sub-populations/strata defined by sample depths, soil types, and other characteristics.

Site data collection requirements depend upon the objective(s) of the study. Specifically, in background versus site comparisons, site data are needed to perform:

- point-by-point onsite comparisons with pre-established ALs or estimated BTVs. Typically, this approach is used when only a small number (e.g., < 6) of onsite observations are compared with a BTV or some other not-to-exceed value. If many onsite values need to be compared with a BTV, the recommended upper limit to use is the UTL or upper simultaneous limit (USL) to control the false positive error rate (Type I Error Rate). More details can be found in Chapter 3 of the Technical Guide. Alternatively, one can use hypothesis testing approaches (Chapter 6 of ProUCL Technical Guide) provided enough observations (at least 10, more are preferred) are available.

- single-sample hypotheses tests to compare site data with a pre-established cleanup standards, C_s (e.g., representing a measure of central tendency); proportion test to compare site proportion of exceedances of an AL with a pre-specified allowable proportion, P_0. These hypotheses testing approaches are used on site data when enough site observations are available. Specifically, when at least 10 (more are desirable) site observations are available; it is preferable to use hypotheses testing approaches to compare site observations with specified threshold values. The use of hypotheses testing approaches can control both types of error rates (Type 1 and Type 2) more efficiently than the point-by-point individual observation comparisons. This is especially true as the number of point-by-point comparisons increases. This issue is illustrated by the following table summarizing the probabilities of exceedances (false positive error rate) of a BTV (e.g., 95th percentile) by onsite observations, even when the site and background populations have comparable distributions. The probabilities of these chance exceedances increase as the site sample size increases.

Sample Size	Probability of Exceedance
1	0.05
2	0.10
5	0.23
8	0.34
10	0.40
12	0.46
64	0.96

- two-sample hypotheses tests to compare site data distribution with background data distribution to determine if the site concentrations are comparable to background concentrations. An adequate amount of data needs to be made available from the site as well as the background populations. It is preferable to collect at least 10 observations from each population under comparison.

Notes: From a mathematical point of view, one can perform hypothesis tests on data sets consisting of only 3-4 data values; however, the reliability of the test statistics (and the conclusions derived) thus obtained is questionable. In these situations it is suggested to supplement the test statistics decisions with graphical displays.

1.3 Discrete Samples or Composite Samples?

ProUCL can be used for discrete sample data sets, as well as on composite sample data sets. However, in a data set (background or site), samples should be either all discrete or all composite. In general, both discrete and composite site samples may be used for individual point-by-point site comparisons with a threshold value, and for single and two-sample hypotheses testing applications.

- When using a single-sample hypothesis testing approach, site data can be obtained by collecting all discrete or all composite samples. The hypothesis testing approach is used when many (≥ 10) site observations are available. Details of the single-sample hypothesis approaches are widely available in EPA guidance documents (MARSSIM 2000, EPA 1989a, 2006b). Several single-sample hypotheses testing procedures available in ProUCL are described in Chapter 6 of the ProUCL 5.1 Technical Guide.

- If a two-sample hypothesis testing approach is used to perform site versus background comparisons, then samples from both of the populations should be either all discrete samples, or all composite samples. The two-sample hypothesis testing approaches are used when many (e.g., at least 10) site, as well as background, observations are available. For better results with higher statistical power, the availability of more observations perhaps based upon an appropriate DQOs process (EPA 2006a) is desirable. Several two-sample hypotheses tests available in ProUCL 5.1 are described in Chapter 6 of the ProUCL 5.1 Technical Guide.

1.4 Upper Limits and Their Use

The computation and use of statistical limits depend upon their applications and the parameters (e.g., EPC term, BTVs) they are supposed to be estimating. Depending upon the objective of the study, a pre-specified cleanup standard, C_s, can be viewed as representing: 1) an average (or median) constituent concentration, μ_0; or 2) a not-to-exceed upper threshold concentration value, A_0. These two threshold values, μ_0, and A_0, represent two significantly different parameters, and different statistical methods and limits are used to compare the site data with these two very different threshold values. Statistical limits, such as a UCL of the population mean, a UPL for an independently obtained "single" observation, or independently obtained "*k*" observations (also called future *k* observations, next *k* observations, or *k* different observations), upper percentiles, and UTLs are often used to estimate the environmental parameters: EPC (μ_0) and a BTV (A_0). A new upper limit, USL was included in ProUCL 5.0 which may be used to estimate a BTV based upon a well-established background data set representing a single statistical population without any outliers.

It is important to understand and note the differences between the uses and numerical values of these statistical limits so that they can be properly used. The differences between UCLs and UPLs (or upper percentiles), and UCLs and UTLs should be clearly understood. A UCL with a 95% confidence limit (UCL95) of the mean represents an estimate of the population mean (measure of the central tendency), whereas a UPL95, a UTL95%-95% (UTL95-95), and an upper 95th percentile represent estimates of a threshold from the upper tail of the population distribution such as the 95th percentile. Here, UPL95 represents a 95% upper prediction limit, and UTL95-95 represents a 95% confidence limit of the 95th percentile. For mildly skewed to moderately skewed data sets, the numerical values of these limits tend to follow the order given as follows.

Sample Mean ≤ UCL95 of Mean ≤ Upper 95th Percentile ≤ UPL95 of a Single Observation ≤ UTL95-95

Example 1-1. Consider a real data set collected from a Superfund site. The data set has several inorganic COPCs, including aluminum (Al), arsenic (As), chromium (Cr), iron (Fe), lead (Pb), manganese (Mn), thallium (Tl) and vanadium (V). Iron concentrations follow a normal distribution. This data set has been used in several examples throughout the two ProUCL guidance documents (Technical Guide and User Guide), therefore it is provided as follows.

Aluminum	Arsenic	Chromium	Iron	Lead	Manganese	Thallium	Vanadium
6280	1.3	8.7	4600	16	39	0.0835	12
3830	1.2	8.1	4330	6.4	30	0.068	8.4
3900	2	11	13000	4.9	10	0.155	11
5130	1.2	5.1	4300	8.3	92	0.0665	9
9310	3.2	12	11300	18	530	0.071	22
15300	5.9	20	18700	14	140	0.427	32
9730	2.3	12	10000	12	440	0.352	19
7840	1.9	11	8900	8.7	130	0.228	17
10400	2.9	13	12400	11	120	0.068	21
16200	3.7	20	18200	12	70	0.456	32
6350	1.8	9.8	7340	14	60	0.067	15
10700	2.3	14	10900	14	110	0.0695	21
15400	2.4	17	14400	19	340	0.07	28
12500	2.2	15	11800	21	85	0.214	25
2850	1.1	8.4	4090	16	41	0.0665	8
9040	3.7	14	15300	25	66	0.4355	24
2700	1.1	4.5	6030	20	21	0.0675	11
1710	1	3	3060	11	8.6	0.066	7.2
3430	1.5	4	4470	6.3	19	0.067	8.1
6790	2.6	11	9230	13	140	0.068	16
11600	2.4	16.4		98.5	72.5	0.13	
4110	1.1	7.6		53.3	27.2	0.068	
7230	2.1	35.5		109	118	0.095	
4610	0.66	6.1		8.3	22.5	0.07	

Several upper limits for iron are summarized as follows, and it be seen that they follow the order (in magnitude) as described above.

Table 1-1. Computation of Upper Limits for Iron (Normally Distributed)

Mean	Median	Min	Max	UCL95	UPL95 for a Single Observation	UPL95 for 4 Observations	UTL95-95	95% Upper Percentile
9618	9615	3060	18700	11478	18145	21618	21149	17534

For highly skewed data sets, these limits may not follow the order described above. This is especially true when the upper limits are computed based upon a lognormal distribution (Singh, Singh, and Engelhardt 1997). It is well known that a lognormal distribution based H-UCL95 (Land's UCL95) often yields unstable and impractically large UCL values. An H-UCL95 often becomes larger than UPL95 and even larger than a UTL 95%-95% and the largest sample value. This is especially true when dealing with skewed data sets of smaller sizes. Moreover, it should also be noted that in some cases, a H-UCL95 becomes smaller than the sample mean, especially when the data are mildly skewed and the sample size is large (e.g., > 50, 100).

There is a great deal of confusion about the appropriate use of these upper limits. A brief discussion about the differences between the applications and uses of the statistical limits described above is provided as follows.

- A UCL represents an average value that is compared with a threshold value also representing an average value (pre-established or estimated), such as a mean C_s. For example, a site 95% UCL exceeding a C_s, may lead to the conclusion that the cleanup standard, C_s has not been attained by the average site area concentration. It should also be noted that UCLs of means are typically computed from the site data set.

- A UCL represents a "collective" measure of central tendency, and it is not appropriate to compare individual site observations with a UCL. Depending upon data availability, single or two-sample hypotheses testing approaches are used to compare a site average or a site median with a specified or pre-established cleanup standard (single-sample hypothesis), or with the background population average or median (two-sample hypothesis).

- A UPL, an upper percentile, or a UTL represents an upper limit to be used for point-by-point individual site observation comparisons. UPLs and UTLs are computed based upon background data sets, and point-by-point onsite observations are compared with those limits. A site observation exceeding a background UTL may lead to the conclusion that the constituent is present at the site at levels greater than the background concentrations level.

- When enough (e.g., at least 10) site observations are available, it is preferable to use hypotheses testing approaches. Specifically, single-sample hypotheses testing (comparing site to a specified threshold) approaches should be used to perform site versus a known threshold comparison; and two-sample hypotheses testing (provided enough background data are also available) approaches should be used to perform site versus background comparison. Several parametric and nonparametric single and two-sample hypotheses testing approaches are available in ProUCL 5.0/ProUCL 5.1.

It is re-emphasized that only averages should be compared with averages or UCLs, and individual site observations should be compared with UPLs, upper percentiles, UTLs, or USLs. For example, the comparison of a 95% UCL of one population (e.g., site) with a 90% or 95% upper percentile of another population (e.g., background) cannot be considered fair and reasonable as these limits (e.g., UCL and UPL) estimate and represent different parameters.

1.5 Point-by-Point Comparison of Site Observations with BTVs, Compliance Limits and Other Threshold Values

The point-by-point observation comparison method is used when a small number (e.g., < 6) of site observations are compared with pre-established or estimated BTVs, screening levels, or preliminary remediation goals (PRGs). Typically, a single exceedance of the BTV by an onsite (or a monitoring well) observation may be considered an indication of the presence of contamination at the site area under investigation. The conclusion of an exceedance by a site value is sometimes confirmed by re-sampling (taking a few more collocated samples) at the site location (or a monitoring well) exhibiting constituent concentrations in excess of the BTV. If all collocated sample observations (or all sample observations collected during the same time period) from the same site location (or well) exceed the BTV or PRG, then it may be concluded that the location (well) requires further investigation (e.g., continuing treatment and monitoring) and possibly cleanup.

When BTV constituent concentrations are not known or pre-established, one has to collect or extract a background data set of an appropriate size that can be considered representative of the site background. Statistical upper limits are computed using the background data set thus obtained, which are used as estimates of BTVs. To compute reasonably reliable estimates of BTVs, a minimum of 10 background observations should be collected, perhaps using an appropriate DQOs process as described in EPA (2000, 2006a). Several statistical limits listed above are used to estimate BTVs based upon a defensible (free of outliers, representing the background population) background data set of an adequate size.

The point-by-point comparison method is also useful when quick turnaround comparisons are required in real time. Specifically, when decisions have to be made in real time by a sampling/screening crew, or when only a few site samples are available, then individual point-by-point site concentrations are compared either with pre-established cleanup goals or with estimated BTVs. The sampling crew can use these comparisons to: 1) screen and identify the COPCs, 2) identify the potentially polluted site AOCs, or 3) continue or stop remediation or excavation at an onsite area of concern.

If a larger number of samples (e.g., >10) are available from the AOC, then the use of hypotheses testing approaches (both single-sample and a two-sample) is preferred. The use of hypothesis testing approaches tends to control the error rates more tightly and efficiently than the individual point-by-point site comparisons.

1.6 Hypothesis Testing Approaches and Their Use

Both single-sample and two-sample hypotheses testing approaches are used to make cleanup decisions at polluted sites, and also to compare constituent concentrations of two (e.g., site versus background) or more populations (e.g., MWs).

1.6.1 Single Sample Hypotheses (Pre-established BTVs and Not-to-Exceed Values are Known)

When pre-established BTVs are used such as the U.S. Geological Survey (USGS) background values (Shacklette and Boerngen 1984), or thresholds obtained from similar sites, there is no need to extract, establish, or collect a background data set. When the BTVs and cleanup standards are known, one-sample hypotheses are used to compare site data (provided enough site data are available) with known and pre-established threshold values. It is suggested that the project team determine (e.g., using DQOs) or decide (depending upon resources) the number of site observations that should be collected and compared with the "pre-established" standards before coming to a conclusion about the status (clean or polluted) of the site AOCs. As mentioned earlier, when the number of available site samples is < 6, one might perform point-by-point site observation comparisons with a BTV; and when enough site observations (at least 10) are available, it is desirable to use single-sample hypothesis testing approaches. Depending upon the parameter (μ_0, A_0), represented by the known threshold value, one can use single-sample hypotheses tests for population mean or median (t-test, sign test), or use single-sample tests for proportions and percentiles. The details of the single-sample hypotheses testing approaches can be found in EPA (2006b) guidance document and in Chapter 6 of ProUCL Technical Guide.

One-Sample t-Test: This test is used to compare the site mean, μ, with some specified cleanup standard, C_s, where the C_s represents an average threshold value, μ_0. The Student's t-test (or a UCL of the mean) is used (assuming normality of site data set or when sample size is large, such as larger than 30, 50) to verify the attainment of cleanup levels at a polluted site after some remediation activities.

One-Sample Sign Test or Wilcoxon Signed Rank (WSR) Test: These tests are nonparametric tests and can also handle ND observations, provided the detection limits of all NDs fall below the specified threshold value, C_s. These tests are used to compare the site location (e.g., median, mean) with some specified C_s representing a similar location measure.

One-Sample Proportion Test or Percentile Test: When a specified cleanup standard, A_0, such as a PRG or a BTV represents an upper threshold value of a constituent concentration distribution rather than the mean threshold value, μ_0, then a test for proportion or a test for percentile (equivalently UTL 95-95 UTL 95-90) may be used to compare site proportion (or site percentile) with the specified threshold or action level, A_0.

1.6.2 Two-Sample Hypotheses (BTVs and Not-to-Exceed Values are Unknown)

When BTVs, not-to-exceed values, and other cleanup standards are not available, then site data are compared directly with the background data. In such cases, two-sample hypothesis testing approaches are used to perform site versus background comparisons. Note that this approach can be used to compare concentrations of any two populations including two different site areas or two different monitoring wells (MWs). In order to use and perform a two-sample hypothesis testing approach, enough data should be available from each of the two populations. Site and background data requirements (e.g., based upon DQOs) for performing two-sample hypothesis test approaches are described in EPA (2000, 2002b, 2006a, 2006b) and also in Chapter 6 of the ProUCL 5.1 Technical Guide. While collecting site and background data, for better representation of populations under investigation, one may also want to account for the size of the background area (and site area for site samples) in sample size determination. That is, a larger number (>15-20) of representative background (and site) samples should be collected from larger background (and site) areas; every effort should be made to collect as many samples as determined by the DQOs-based sample sizes.

The two-sample (or more) hypotheses approaches are used when the site parameters (e.g., mean, shape, distribution) are being compared with the background parameters (e.g., mean, shape, distribution). The two-sample hypotheses testing approach is also used when the cleanup standards or screening levels are not known *a priori*. Specifically, in environmental applications, two-sample hypotheses testing approaches are used to compare average or median constituent concentrations of two or more populations. To derive reliable conclusions with higher statistical power based upon hypothesis testing approaches, an adequate amount of data (e.g., minimum of 10 samples) should be collected from all of the populations under investigation.

The two-sample hypotheses testing approaches incorporated in ProUCL 5.1 are listed as follows:

1. Student t-test (with equal and unequal variances) – Parametric test assumes normality
2. Wilcoxon-Mann-Whitney (WMW) test – Nonparametric test handles data with NDs with one DL - assumes two populations have comparable shapes and variability
3. Gehan test – Nonparametric test handles data sets with NDs and multiple DLs - assumes comparable shapes and variability
4. Tarone-Ware (T-W) test – Nonparametric test handles data sets with NDs and multiple DLs - assumes comparable shapes and variability

The Gehan and T-W tests are meant to be used on left-censored data sets with multiple DLs. For best results, the samples collected from the two (or more) populations should all be of the same type obtained using similar analytical methods and apparatus; the collected site and background samples should all be discrete or all composite (obtained using the same design and pattern), and be collected from the same medium (soil) at similar depths (e.g., all surface samples or all subsurface samples) and time (e.g., during the same quarter in groundwater applications) using comparable (preferably same) analytical methods. Good sample collection methods and sampling strategies are given in EPA (1996, 2003) guidance documents.

Note: ProUCL 5.1 (and previous versions) has been developed using limited government funding. ProUCL 5.1 is equipped with statistical and graphical methods needed to address many environmental sampling and statistical issues as described in the various CERCLA, MARSSIM, and RCRA documents cited earlier. However, one may not compare the availability of methods in ProUCL 5.1 with methods incorporated in commercial software packages such as SAS® and Minitab 16. Not all methods available in the statistical literature are available in ProUCL.

1.7 Minimum Sample Size Requirements and Power Evaluations

Due to resource limitations, it is not be possible (nor needed) to sample the entire population (e.g., background area, site area, AOCs, EAs) under study. Statistics is used to draw inference(s) about the populations (clean, dirty) and their known or unknown statistical parameters (e.g., mean, variance, upper threshold values) based upon much smaller data sets (samples) collected from those populations. To determine and establish BTVs and site specific screening levels, defensible data set(s) of appropriate size(s) representing the background population (e.g., site-specific, general reference area, or historical data) need to be collected. The project team and site experts should decide what represents a site population and what represents a background population. The project team should determine the population area and boundaries based upon all current and intended future uses, and the objectives of data collection. Using the collected site and background data sets, statistical methods supplemented with graphical displays are used to perform site versus background comparisons. The test results and statistics obtained by performing such site versus background comparisons are used to determine if the site and background level constituent concentrations are comparable; or if the site concentrations exceed the background threshold concentration level; or if an adequate amount of remediation approaching the BTV or some cleanup level has been performed at polluted site AOCs.

To perform these statistical tests, determine the number of samples that need to be collected from the populations (e.g., site and background) under investigation using appropriate DQOs processes (EPA 2000, 2006a, 2006b). ProUCL has the **Sample Sizes** module which can be used to develop DQOs based sampling designs needed to address statistical issues associated with polluted sites projects. ProUCL provides user-friendly options to enter the desired/pre-specified values of decision parameters (e.g., Type I and Type II error rates) to determine minimum sample sizes for the selected statistical applications including: estimation of mean, single and two-sample hypothesis testing approaches, and acceptance sampling. Sample size determination methods are available for the sampling of continuous characteristics (e.g., lead or Radium 226), as well as for attributes (e.g., proportion of occurrences exceeding a specified threshold). Both parametric (e.g., t-tests) and nonparametric (e.g., Sign test, test for proportions, WRS test) sample size determination methods are available in ProUCL 5.1 and in its earlier versions (e.g., ProUCL 4.1). ProUCL also has sample size determination methods for acceptance sampling of lots of discrete objects such as a batch of drums containing hazardous waste (e.g., RCRA applications, U.S. EPA 2002c).

However, due to budgetary or logistical constraints, it may not be possible to collect the same number of samples as determined by applying a DQO process. For example, the data might have already been collected (as often is the case) without using a DQO process, or due to resource constraints, it may not have been possible to collect as many samples as determined by using a DQO-based sample size formula.

In practice, the project team and the decision makers tend not to collect enough background samples. It is suggested to collect at least 10 background observations before using statistical methods to perform background evaluations based upon data collected using discrete samples. The minimum sample size recommendations described here are useful when resources are limited, and it may not be possible to collect as many background and site samples as computed using DQOs based sample size determination formulae. In case data are collected without using a DQO process, the **Sample Sizes** module can be used to assess the power of the test statistic in retrospect. Specifically, one can use the standard deviation of the computed test statistic (EPA 2006b) and compute the sample size needed to meet the desired DQOs. If the computed sample size is greater than the size of the data set used, the project team may want to collect additional samples to meet the desired DQOs.

<u>Note:</u> From a mathematical point of view, the statistical methods incorporated in ProUCL and described in this guidance document for estimating EPC terms and BTVs, and comparing site versus background concentrations can be performed on small site and background data sets (e.g., of sizes as small as 3). However, those statistics may not be considered representative and reliable enough to make important cleanup and remediation decisions which will potentially impact human health and the environment. ProUCL provides messages when the number of detects is <4-5, and suggests collecting at least 8-10 observations. Based upon professional judgment, as a rule-of-thumb, ProUCL guidance documents recommend collecting a minimum of 10 observations when data sets of a size determined by a DQOs process (EPA 2006) cannot be collected. This however, should not be interpreted as the general recommendation and every effort should be made to collect DQOs based number of samples. Some recent guidance documents (e.g., EPA 2009) have also adopted this rule-of-thumb and suggest collecting a minimum of about 8-10 samples in the circumstance that data cannot be collected using a DQO-based process. However, the project team needs to make these determinations based upon their comfort level and knowledge of site conditions.

- To allow users to compute decision statistics using data from ISM (ITRC, 2012) samples, ProUCL 5.1 will compute decision statistics (e.g., UCLs, UPLs, UTLs) based upon samples of sizes as small as 3. The user is referred to the ITRC ISM Technical Regulatory Guide (2012) to determine which UCL (e.g., Student's t-UCL or Chebyshev UCL) should be used to estimate the EPC term.

1.7.1 Why a data set of minimum size, n = 8-10?

Typically, the computation of parametric upper limits (UPL, UTL, UCL) depends upon three values: the sample mean, sample variability (standard deviation) and a critical value. A critical value depends upon sample size, data distribution, and confidence level. For samples of small size (< 8-10), the critical values are large and unstable, and upper limits (e.g., UTLs, UCLs) based upon a data set with fewer than 8-10 observations are mainly driven by those critical values. The differences in the corresponding critical values tend to stabilize when the sample size becomes larger than 8-10 (see tables below, where degrees of freedom [*df*] = sample size - 1). This is one of the reasons ProUCL guidance documents suggest a minimum data set size of 10 when the number of observations determined from sample-size calculations based upon EPA DQO process exceed the logistical/financial/temporal/constraints of a project. For samples of sizes 2-11, 95% critical values used to compute upper limits (UCLs, UPLs, UTLs, and USLs) based upon a normal distribution are summarized in the subsequent tables. In general, a similar pattern is followed for critical values used in the computation of upper limits based upon other distributions.
For the normal distribution, Student's t-critical values are used to compute UCLs and UPLs which are summarized as follows.

Table of Critical Values of t-Statistic
df= sample size-1= *(n-1)*

	Upper-tail probability *p*				
df	.10	.05	.025	.02	.01
1	3.078	6.314	12.71	15.89	31.82
2	1.886	2.920	4.303	4.849	6.965
3	1.638	2.353	3.182	3.482	4.541
4	1.533	2.132	2.776	2.999	3.747
5	1.476	2.015	2.571	2.757	3.365
6	1.440	1.943	2.447	2.612	3.143
7	1.415	1.895	2.365	2.517	2.998
8	1.397	1.860	2.306	2.449	2.896
9	1.383	1.833	2.262	2.398	2.821
10	1.372	1.812	2.228	2.359	2.764

One can see that once the sample size starts exceeding 9-10 (*df* = 8, 9), the difference between the critical values starts stabilizing. For example, for upper tail probability (= level of significance) of 0.05, the difference between critical values for *df* = 9 and *df* =10 is only 0.021, where as the difference between critical values for *df*= 4 and 5 is 0.117; similar patterns are noted for other levels of significance. For the normal distribution, critical values used to compute UTL90-95, UTL95-95, USL90, and USL95 are described as follows. One can see that once the sample size starts exceeding 9-10, the difference between the critical values starts decreasing significantly.

n	UTL90-95	UTL95-95	USL90	USL95
3	6.155	7.656	1.148	1.153
4	4.162	5.144	1.425	1.462
5	3.407	4.203	1.602	1.671
6	3.006	3.708	1.729	1.822
7	2.755	3.399	1.828	1.938
8	2.582	3.187	1.909	2.032
9	2.454	3.031	1.977	2.11
10	2.355	2.911	2.036	2.176
11	2.275	2.815	2.088	2.234

Note: Nonparametric upper limits (UPLs, UTLs, and USLs) are computed using higher order statistics of a data set. To achieve the desired confidence coefficient, samples of sizes much greater than 10 are required. For details, refer to Chapter 3. It should be noted that critical values of USLs are significantly lower than critical values for UTLs. Critical values associated with UTLs decrease as the sample size increases. Since, as the sample size increases the maximum of the data set also increases, and critical values associated with USLs increase with the sample size.

1.7.2 Sample Sizes for Bootstrap Methods

Several nonparametric methods including bootstrap methods for computing UCL, UTL, and other limits for both full-uncensored data sets and left-censored data sets with NDs are available in ProUCL 5.1. Bootstrap resampling methods are useful when not too few (e.g., < 15-20) and not too many (e.g., > 500-1000) observations are available. For bootstrap methods (e.g., percentile method, BCA bootstrap method, bootstrap-t method), a large number (e.g., 1000, 2000) of bootstrap resamples are drawn with replacement from the same data set. Therefore, to obtain bootstrap resamples with at least some distinct values (so that statistics can be computed from each resample), it is suggested that a bootstrap method should not be used when dealing with small data sets of sizes less than 15-20. Also, it is not necessary to bootstrap a large data set of size greater than 500 or 1000; that is when a data set of a large size (e.g., > 500) is available, there is no need to obtain bootstrap resamples to compute statistics of interest (e.g., UCLs). One can simply use a statistical method on the original large data set.

Note: Rules-of-thumb about minimum sample size requirements described in this section are based upon professional experience of the developers. ProUCL software is not a policy software. It is recommended that the users/project teams/agencies make determinations about the minimum number of observations and minimum number of detects that should be present in a data set before using a statistical method.

1.8 Statistical Analyses by a Group ID

The analyses of data categorized by a group ID variable such as: 1) Surface vs. Subsurface; 2) AOC1 vs. AOC2; 3) Site vs. Background; and 4) Upgradient vs. Downgradient monitoring wells are common in environmental applications. ProUCL 5.1 offers this option for data sets with and without NDs. The **Group Option** provides a tool for performing separate statistical tests and for generating separate graphical displays for each member/category of the group (samples from different populations) that may be present in a data set. The graphical displays (e.g., box plots, quantile-quantile plots) and statistics (e.g., background statistics, UCLs, hypotheses tests) of interest can be computed separately for each group by using this option. Moreover, using the **Group Option**, graphical methods can display multiple graphs (e.g., Q-Q plots) on the same graph providing graphical comparison of multiple groups.

It should be pointed out that it is the user's responsibility to provide an adequate amount of data to perform the group operations. For example, if the user desires to produce a graphical Q-Q plot (e.g., using only detected data) with regression lines displayed, then there should be at least two detected data values (to compute slope, intercept, *sd*) in the data set. Similarly, if the graphs are desired for each group specified by the group ID variable, there should be at least two observations in each group specified by the group variable. When ProUCL data requirements are not met, ProUCL does not perform any computations, and generates a warning message (colored orange) in the lower Log Panel of the output screen of ProUCL 5.1.

1.9 Statistical Analyses for Many Constituents/Variables

ProUCL software can process multiple analytes/variables simultaneously in a user-friendly manner This option is useful when one has to process multiple variables and compute decision statistics (e.g., UCLs, UPLs, and UTLs) and test statistics (e.g., ANOVA test, trend test) for multiple variables. It is the user's responsibility to make sure that each selected variable has an adequate amount of data so that ProUCL can perform the selected statistical method correctly. ProUCL displays warning messages when a selected variable does not have enough data needed to perform the selected statistical method.

1.10 Use of Maximum Detected Value as Estimates of Upper Limits

Some practitioners use the maximum detected value as an estimate of the EPC term. This is especially true when the sample size is small such as < 5, or when a UCL95 exceeds the maximum detected values (EPA 1992a). Also, many times in practice, the BTVs and not-to-exceed values are estimated by the maximum detected value (e.g., nonparametric UTLs, USLs).

1.10.1 Use of Maximum Detected Value to Estimate BTVs and Not-to-Exceed Values

BTVs and not-to-exceed values represent upper threshold values from the upper tail of a data distribution; therefore, depending upon the data distribution and sample size, the BTVs and other not-to-exceed values may be estimated by the largest or the second largest detected value. A nonparametric UPL, UTL, and USL are often estimated by higher order statistics such as the maximum value or the second largest value (EPA 1992b, 2009, Hahn and Meeker 1991). The use of higher order statistics to estimate the UTLs depends upon the sample size. For data sets of size: 1) 59 to 92 observations, a nonparametric UTL95-95 is given by the maximum detected value; 2) 93 to 123 observations, a nonparametric UTL95-95 is given by the second largest maximum detected value; and 3) 124 to 152 observations, a UTL95-95 is given by the third largest detected value in the sample, and so on.

1.10.2 Use of Maximum Detected Value to Estimate EPC Terms

Some practitioners tend to use the maximum detected value as an estimate of the EPC term. This is especially true when the sample size is small such as < 5, or when a UCL95 exceeds the maximum detected value. Specifically, the EPA (1992a) document suggests the use of the maximum detected value as a default value to estimate the EPC term when a 95% UCL (e.g., the H-UCL) exceeds the maximum value in a data set. ProUCL computes 95% UCLs of the mean using several methods based upon normal, gamma, lognormal, and non-discernible distributions. In the past, a lognormal distribution was used as the default distribution to model positively skewed environmental data sets. Additionally, only two methods were used to estimate the EPC term based upon: 1) normal distribution and Student's t-statistic, and 2) lognormal distribution and Land's H-statistic (Land 1971, 1975). The use of the H-statistic often yields unstable and impractically large UCL95 of the mean (Singh, Singh, and Engelhardt 1997; Singh, Singh, and Iaci 2002). For highly skewed data sets of smaller sizes (< 30, < 50), H-UCL often exceeds the maximum detected value. Since the use of a lognormal distribution has been quite common (suggested as a default model in the risk assessment guidance for Superfund [RAGS] document [EPA 1992a]), the exceedance of the maximum value by an H-UCL95 is frequent for many skewed data sets of smaller sizes (e.g., < 30, < 50). These occurrences result in the possibility of using the maximum detected value as an estimate of the EPC term.

It should be pointed out that in some cases, the maximum observed value actually might represent an impacted location. Obviously, it is not desirable to use an observation potentially representing an impacted location to estimate the EPC for an AOC. The EPC term represents the average exposure contracted by an individual over an EA during a long period of time; the EPC term should be estimated by using an average value (such as an appropriate 95% UCL of the mean) and not by the maximum observed concentration. One needs to compute an average exposure and not the maximum exposure. Singh and Singh (2003) studied the performance of the max test (using the maximum observed value to estimate the EPC) via Monte Carlo simulation experiments. They noted that for skewed data sets of small sizes (e.g., < 10-20), even the max test does not provide the specified 95% coverage to the population mean, and for larger data sets it overestimates the EPC term, which may lead to unnecessary further remediation.

Several methods, some of which are described in EPA (2002a) and other EPA documents, are available in versions of ProUCL (i.e., ProUCL 3.00.02 [EPA 2004], ProUCL 4.0 [U.S. EPA 2007], ProUCL 4.00.05 [EPA 2009, 2010], ProUCL 4.1 [EPA 2011]) for estimating the EPC terms. For data sets with NDs, ProUCL 5.0 (and ProUCL 5.1) has some new UCL (and other limits) computation methods which were not available in earlier versions of ProUCL. It is unlikely that the UCLs based upon those methods will exceed the maximum detected value, unless some outliers are present in the data set.

1.10.2.1 Chebyshev Inequality Based UCL95

ProUCL 5.1 (and its earlier versions) displays a warning message when the suggested 95% UCL (e.g., Hall's or bootstrap-t UCL with outliers) of the mean exceeds the detected maximum concentration. When a 95% UCL does exceed the maximum observed value, ProUCL suggests the use of an alternative UCL computation method based upon the Chebyshev inequality. One may use a 97.5% or 99% Chebyshev UCL to estimate the mean of a highly skewed population. The use of the Chebyshev inequality to compute UCLs tends to yield more conservative (but stable) UCLs than other methods available in ProUCL software. In such cases, when the sample size is large (and other UCL methods such as the bootstrap-t method yield unrealistically high values due to presence of outliers), one may want to use a 95% Chebyshev UCL or a Chebyshev UCL with a lower confidence coefficient such as 90% as an estimate of the population mean, especially when the sample size is large (e.g., >100, 150). The details (as functions of sample size and skewness) for the use of those UCLs are summarized in various versions of ProUCL Technical Guides (EPA 2004, 2007, 2009, 2010d, 2011, 2013a).

Notes: Using the maximum observed value to estimate the EPC term representing the average exposure contracted by an individual over an EA is not recommended. For the sake of interested users, ProUCL displays a warning message when the recommended 95% UCL (e.g., Hall's bootstrap UCL) of the mean exceeds the observed maximum concentration. For such scenarios (when a 95% UCL does exceed the maximum observed value), an alternative UCL computation method based upon Chebyshev inequality is suggested by the ProUCL software.

1.11 Samples with Nondetect Observations

ND observations are inevitable in most environmental data sets. Singh, Maichle, and Lee (2006) studied the performances (in terms of coverages) of the various UCL95 computation methods including the simple substitution methods (such as the DL/2 and DL methods) for data sets with ND observations. They concluded that the UCLs obtained using the substitution methods, including the replacement of NDs by DL/2; do not perform well even when the percentage of ND observations is low, such as less than 5% to 10%. They recommended avoiding the use of substitution methods for computing UCL95 based upon data sets with ND observations.

1.11.1 Avoid the Use of the DL/2 Substitution Method to Compute UCL95

Based upon the results of the report by Singh, Maichle, and Lee (2006), it is recommended to avoid the use of the DL/2 substitution method when performing a GOF test, and when computing the summary statistics and various other limits (e.g., UCL, UPL, UTLs) often used to estimate the EPC terms and BTVs. Until recently, the substitution method has been the most commonly used method for computing various statistics of interest for data sets which include NDs. The main reason for this has been the lack of the availability of the other rigorous methods and associated software programs that can be used to estimate the various environmental parameters of interest. Today, several methods (e.g., using KM estimates) with better performance, including the Chebyshev inequality and bootstrap methods, are available for computing the upper limits of interest. Several of those parametric and nonparametric methods are available in ProUCL 4.0 and higher versions. The DL/2 method is included in ProUCL for historical reasons as it had been the most commonly used and recommended method until recently (EPA 2006b). EPA scientists and several reviewers of the ProUCL software had suggested and requested the inclusion of the DL/2 substitution method in ProUCL for comparison and research purposes.

Notes: Even though the DL/2 substitution method has been incorporated in ProUCL, its use is **not recommended** due to its poor performance. The DL/2 substitution method has been retained in ProUCL 5.1 for historical and comparison purposes. NERL-EPA, Las Vegas strongly recommends avoiding the use of this method even when the percentage of NDs is as low as 5% to 10%.

1.11.2 ProUCL Does Not Distinguish between Detection Limits, Reporting limits, or Method Detection Limits

ProUCL 5.1 (and all previous versions) does not make distinctions between method detection limits (MDLs), adjusted MDLs, sample quantitation limits (SQLs), reporting limits (RLs), or DLs. Multiple DLs (or RLs) in ProUCL mean different values of the detection limits. It is user's responsibility to understand the differences between these limits and use appropriate values (e.g., DLs) for nondetect values below which the laboratory cannot reliably detect/measure the presence of the analyte in collected samples (e.g., soil samples). A data set consisting of values less than the DLs (or MDLs, RLs) is considered a left-censored data set. ProUCL uses statistical methods available in the statistical literature for left-censored data sets for computing statistics of interest including mean, *sd*, UCL, and estimates of BTVs.

The user determines which qualifiers (e.g., J, U, UJ) will be considered as nondetects. Typically, all values with U or UJ qualifiers are considered as nondetect values. It is the user's responsibility to enter a value which can be used to represent a ND value. For NDs, the user enters the associated DLs or RLs (and not zeros or half of the detection limits). An indicator column/variable, D_x taking a value, 0, for all nondetects and a value, 1, for all detects is assigned to each variable, x, with NDs. It is the user's responsibility to supply the numerical values for NDs (should be entered as reported DLs) not qualifiers (e.g., J, U, B, UJ). For example, for thallium with nondetect values, the user creates an associated column labeled as D_thallium to tell the software that the data set will have nondetect values. This column, D_thallium consists of only zeros (0) and ones (1); zeros are used for all values reported as NDs and ones are used for all values reported as detects.

1.12 Samples with Low Frequency of Detection

When all of the sampled values are reported as NDs, the EPC term and other statistical limits should also be reported as a ND value, perhaps by the maximum RL or the maximum RL/2. The project team will need to make this determination. Statistics (e.g., UCL95) based upon only a few detected values (e.g., < 4) cannot be considered reliable enough to estimate EPCs which can have a potential impact on human health and the environment. When the number of detected values is small, it is preferable to use ad hoc methods rather than using statistical methods to compute EPCs and other upper limits. Specifically, for data sets consisting of < 4 detects and for small data sets (e.g., size < 10) with low detection frequency (e.g., < 10%), the project team and the decision makers should decide, on a site-specific basis, how to estimate the average exposure (EPC) for the constituent and area under consideration. For data sets with low detection frequencies, other measures such as the median or mode represent better estimates (with lesser uncertainty) of the population measure of central tendency.

Additionally, when most (e.g., > 95%) of the observations for a constituent lie below the DLs, the sample median or the sample mode (rather than the sample average) may be used as an estimate of the EPC. Note that when the majority of the data are NDs, the median and the mode may also be represented by a ND value. The uncertainty associated with such estimates will be high. The statistical properties, such as the bias, accuracy, and precision of such estimates, would remain unknown. In order to be able to compute defensible estimates, it is always desirable to collect more samples.

1.13 Some Other Applications of Methods in ProUCL 5.1

In addition to performing background versus site comparisons for CERCLA and RCRA sites, performing trend evaluations based upon time-series data sets, and estimating EPCs in exposure and risk evaluation studies, the statistical methods in ProUCL can be used to address other issues dealing with environmental investigations that are conducted at Superfund or RCRA sites.

1.13.1 Identification of COPCs

Risk assessors and remedial project managers (RPMs) often use screening levels or BTVs to identify COPCs during the screening phase of a cleanup project at a contaminated site. The screening for COPCs is performed prior to any characterization and remediation activities that are conducted at the site. This comparison is performed to screen out those constituents that may be present in the site medium of interest at low levels (e.g., at or below the background levels or some pre-established screening levels) and may not pose any threat and concern to human health and the environment. Those constituents may be eliminated from all future site investigations, and risk assessment and risk management studies.

To identify the COPCs, point-by-point site observations are compared with some pre-established soil screening levels (SSL) or estimated BTVs. This is especially true when the comparisons of site concentrations with screening levels or BTVs are conducted in real time by the sampling or cleanup crew onsite. The project team should decide the type of site samples (discrete or composite) and the number of site observations that should be collected and compared with the screening levels or the BTVs. In case BTVs or screening levels are not known, the availability of a defensible site-specific background or reference data set of reasonable size (e.g., at least 10) is required for computing reliable and representative estimates of BTVs and screening levels. The constituents with concentrations exceeding the respective screening values or BTVs may be considered COPCs, whereas constituents with concentrations (e.g., in all collected samples) lower than the screening values or BTVs may be omitted from all future evaluations.

1.13.2 Identification of Non-Compliance Monitoring Wells

In MW compliance assessment applications, individual (often discrete) constituent concentrations from a MW are compared with some pre-established limits such as an ACL or a maximum concentration limit (MCL). An exceedance of the MCL or the BTV (e.g., estimated by a UTL95-95 or a UPL95) by a MW concentration may be considered an indication of contamination in that MW. For individual concentration comparisons, the presence of contamination (determined by an exceedance) may have to be confirmed by re-sampling from that MW. If concentrations of constituents in the original sample and re-sample(s) exceed the MCL or BTV, then that MW may require further scrutiny, perhaps triggering remediation activities. If the concentration data from a MW for 4 to 5 continuous quarters (or some other designated time period determined by the project team) are below the MCL or BTV level, then that MW may be considered as complying with (achieving) the pre-established or estimated standards.

1.13.3 Verification of the Attainment of Cleanup Standards, C_s

Hypothesis testing approaches are used to verify the attainment of the cleanup standard, C_s, at site AOCs after conducting remediation and cleanup at those site AOCs (EPA 1989a, 1994). In order to assess the attainment of cleanup levels, a representative data set of adequate size perhaps obtained using the DQO process (or a minimum of 10 observations should be collected) needs to be made available from the remediated/excavated areas of the site under investigation. The sample size should also account for the size of the remediated site areas: meaning that larger site areas should be sampled more (with more observations) to obtain a representative sample of the remediated areas under investigation. Typically, the null hypothesis of interest is H_0: Site Mean, $\mu_s \geq C_s$ versus the alternative hypothesis, H_1: Site Mean, $\mu_s < C_s$, where the cleanup standard, C_s, is known *a priori*.

1.13.4 Using BTVs (Upper Limits) to Identify Hot Spots

The use of upper limits (e.g., UTLs) to identify hot spot(s) has also been mentioned in the *Guidance for Comparing Background and Chemical Concentrations in Soil for CERCLA Sites* (EPA 2002b). Point-by-point site observations are compared with a pre-established or estimated BTV. Exceedances of the BTV by site observations may represent impacted locations with elevated concentrations (hot spots).

1.14 Some General Issues, Suggestions and Recommendations made by ProUCL

Some general issues regarding the handling of multiple DLs by ProUCL and recommendations made about various substitution and ROS methods for data sets with NDs are described in the following sections.

1.14.1 Handling of Field Duplicates

ProUCL does not pre-process field duplicates. The project team determines how field duplicates will be handled and pre-processes the data accordingly. For an example, if the project team decides to use average values for field duplicates, then averages need to be computed and field duplicates need to be replaced by their respective average values. It is the user's responsibility to feed in appropriate values (e.g., averages, maximum) for field duplicates. The user is advised to refer to the appropriate EPA guidance documents related to collection and use of field duplicates for more information.

1.14.2 ProUCL Recommendation about ROS Method and Substitution (DL/2) Method

For data sets with NDs, ProUCL can compute point estimates of population mean and standard deviation using the KM and ROS methods (and also using the DL/2 substitution method). The substitution method has been retained in ProUCL for historical and research purposes. ProUCL uses Chebyshev inequality, bootstrap methods, and normal, gamma, and lognormal distribution based equations on KM (or ROS) estimates to compute upper limits (e.g., UCLs, UTLs). The simulation study conducted by Singh, Maichle and Lee (2006) demonstrated that the KM method yields accurate estimates of the population mean. They also demonstrated that for moderately skewed to highly skewed data sets, UCLs based upon KM estimates and BCA bootstrap (mild skewness), KM estimates and Chebyshev inequality (moderate to high skewness), and KM estimates and bootstrap-t method (moderate to high skewness) yield better (in terms of coverage probability) estimates of EPCs than other UCL methods based upon the Student's t-statistic on KM estimates, percentile bootstrap method on KM or ROS estimates.

1.14.3 Unhandled Exceptions and Crashes in ProUCL

A typical statistical software, especially developed under limited resources may not be able to accommodate data sets with all kinds of deficiencies such as all missing values for a variable, or all nondetect values for a variable. An inappropriate/insufficient data set can occur in various forms and not all of them can be addressed in a scientific program like ProUCL. Specifically, from a programming point of view, it can be quite burdensome on the programmer to address all potential deficiencies that can occur in a data set. ProUCL 5.1 addresses many data deficiencies and produces warming messages. All data deficiencies causing unhandled exceptions which were identified by users have been addressed in ProUCL 5.1. However, when ProUCL yields an unhandled exception or crashes, it is highly likely that there is something wrong with the data set; the user is advised to review the input data set to make sure that the data set follows ProUCL data and formatting requirements.

1.15 The Unofficial User Guide to ProUCL4 (Helsel and Gilroy 2012)

Several ProUCL 4.1 users sent inquiries about the validity of the comments made about the ProUCL software in the Unofficial User Guide to ProUCL4 (Helsel and Gilroy, 2012) and in the Practical Stats webinar, "ProUCL v4: The Unofficial User Guide," presented by Dr. Helsel on October 15, 2012 (Helsel 2012a). Their inquiries led us to review comments made about the ProUCL4 software and its associated guidance documents (EPA 2007, 2009a, 2009b, 2010c, 2010d, and 2011) in the "The Unofficial Users Guide to ProUCL4" and in the webinar, "ProUCL v4: The Unofficial User Guide". These two documents collectively are referred to as the Unofficial ProUCLv4 User Guide in this ProUCL document. The pdf document describing the material presented in the Practical Stats Webinar (Helsel 2012a) was downloaded from the http://www.practicalstats.com website.

In the "ProUCL v4: The Unofficial User Guide", comments have been made about the software and its guidance documents, therefore, it is appropriate to address those comments in the present ProUCL guidance document. It is necessary to provide the detailed response to assure that: 1) rigorous statistical methods are used to compute decision making statistics; and 2) the methods incorporated in ProUCL software are not misrepresented and misinterpreted. Some general responses and comments about the material presented in the webinar and in the Unofficial User Guide to ProUCLv4 are described as follows. Specific comments and responses are also considered in the respective chapters of ProUCL 5.1 (and ProUCL 5.0) guidance documents.

Note: It is noted that the Kindle version of "ProUCL v4: Unofficial User Guide" is no longer available on Amazon. Several incorrect theoretical statements and statements misrepresenting ProUCL 4 were made in that Unofficial User Guide; therefore, a brief response to some of those statements has been retained in ProUCL 5.1 guidance documents.

ProUCL is a freeware software package which has been developed under limited government funding to address statistical issues associated with various environmental site projects. Not all statistical methods (e.g., Levene test) described in the statistical literature have been incorporated in ProUCL. One should not compare ProUCL with commercial software packages which are expensive and not as user-friendly as the ProUCL software when addressing environmental statistical issues. The existing and some new statistical methods based upon the research conducted by ORD-NERL, EPA Las Vegas during the last couple of decades have been incorporated in ProUCL to address the statistical needs of various environmental site projects and research studies. Some of those new methods may not be available in text books, in the library of programs written in R-script, and in commercial software packages. However, those methods are described in detail in the cited published literature and also in the ProUCL Technical Guides (e.g., EPA 2007, 2009a, 2009b, 2010c, 2010d, and 2011). Even though for uncensored data sets, programs which compute gamma distribution based UCLs and UPLs are available in R Script, programs which compute a 95% UCL of mean based upon a gamma distribution on KM estimates are not as easily available.

- In the Unofficial ProUCL v4 User Guide, several statements have been made about percentiles. There are several ways to compute percentiles. Percentiles computed by ProUCL may or may not be identical (don't have to be) to percentiles computed by NADA for R (Helsel 2013) or described in Helsel and Gilroy (2012). To address users' requests, ProUCL 4.1 (2011) and its higher versions compute percentiles that are comparable to the percentiles computed by Excel 2003 and higher versions.

- The literature search suggests that there are a total of nine (9) known types of percentiles, i.e., 9 different methods of calculating percentiles in statistics literature (Hyndman and Fan, 1996). The R programming language (R Core Team 2012) computes percentiles using those 9 methods using the following statement in R

  Quantile (x, p, type=k) where p = percentile, k = integer between 1 - 9

  ProUCL computes percentiles using Type 7; Minitab 16 and SPSS compute percentiles using Type 6. It is simply a matter of choice, as there is no 'best' type to use. Many software packages use one type for calculating a percentile, and another for generating a box plot (Hyndman and Fan 1996).

- An incorrect statement "*By definition, the sample mean has a 50% chance of being below the true population mean"* has been made in Helsel and Gilroy (2012) and also in Helsel (2012a). The above statement is not correct for means of skewed distributions (e.g., lognormal or gamma) commonly occurring in environmental applications. Since Helsel (2012) prefers to use a lognormal distribution, the incorrectness of the above statement has been illustrated using a lognormal distribution. The mean and median of a lognormal distribution (details in Section 2.3.2 of Chapter 2 of ProUCL 5.1 Technical Guide) are given by:

  $$\text{mean} = \mu_1 = \exp(\mu + 0.5\sigma^2)\text{; and median} = M = \exp(\mu)$$

  From the above equations, it is clear that the mean of a lognormal distribution is always greater than the median for all positive values of σ (*sd* of log-transformed variable). Actually the mean is greater than the p^{th} percentile when $\sigma > 2z_p$. For example, when $p = 0.80$, $z_p = 0.845$, and mean of a lognormal distribution, μ_1 exceeds $x_{0.80}$, the 80[th] percentile when $\sigma > 1.69$. In other words, when $\sigma > 1.69$ the lognormal mean will exceed the 80[th] percentile of a lognormal distribution. Here z_p represents the p^{th} percentile of the standard normal distribution (SND) with mean 0 and variance 1.

  To demonstrate the incorrectness of the above statement, a small simulation study was conducted. The distribution of sample means based upon samples of size 100 were generated from lognormal distributions with $\mu = 4$, and varying skewness. The experiment was performed 10,000 times to generate the distributions of sample means. The probabilities of sample means less than the population means were computed. The following results are noted.

Table 1-2. Probabilities $p(\bar{x} < \mu_1)$ Computed for Lognormal Distributions with μ=4 and Varying Values of σ

Results are based upon 10000 Simulation Runs for Each Lognormal Distribution Considered

Parameter	**μ=4, σ=0.5 μ_1=61.86 σ_1=32.97**	**μ=4, σ=1 μ_1=90.017 σ_1=117.997**	**μ=4,σ=1.5 μ_1=168.17 σ_1=489.95**	**μ=4,σ=2 μ_1=403.43 σ_1=2953.53**	**μ=4,σ=2.5 μ_1=1242.65, σ_1=28255.23**
$p(\bar{x} < \mu_1)$	**0.519**	**0.537**	**0.571**	**0.651**	**0.729**
Mean	61.835	89.847	168.70	405.657	1193.67
Median	61.723	89.003	160.81	344.44	832.189

The probabilities summarized in the above table demonstrate that the statement about the mean made in Helsel and Gilroy (2012) is incorrect.

- Graphical Methods: Graphical methods are available in ProUCL as exploratory tools which can be generated for both uncensored and left-censored data sets. Exploratory graphical methods are used to understand possible patterns present in data sets and not to compute statistics used in the decision making process. The Unofficial ProUCL Guide makes several comments about box plots and Q-Q plots incorporated in ProUCL. The Unofficial ProUCL Guide states that all graphs with NDs are incorrect. These statements are misleading and incorrect. The intent of the graphical methods in ProUCL is exploratory for the purpose of gaining information (e.g., outliers, multiple populations, data distribution, patterns, and skewness) about a data set. Based upon the data displayed (ProUCL displays a message [e.g., as a sub-title] in this regard) on those graphs, all statistics shown on those graphs generated by ProUCL are correct.

- Box Plots: In statistical literature, one can find several ways to generate box plots. The practitioners may have their own preferences to use one method over the other. All box plot methods including the one in ProUCL convey the same information about the data set (outliers, mean, median, symmetry, skewness). ProUCL uses a couple of development tools such as FarPoint spread (for Excel type input and output operations) and ChartFx (for graphical displays); and ProUCL generates box plots using the built-in box plot feature in ChartFx. For all practical and exploratory purposes, box plots in ProUCL are equally good (if not better) as those available in the various commercial software packages, for examining data distribution (skewed or symmetric), identifying outliers, and comparing multiple groups (main objectives of box plots in ProUCL).

    - As mentioned earlier, it is a matter of choice of using percentiles/quartiles to construct a box plot. There is no 'best' method for constructing a box plot. Many software packages use one method (out of 9 as specified above) for calculating a percentile, and another for constructing a box plot (Hyndman and Fan 1996).

- Q-Q plots: All Q-Q plots incorporated in ProUCL are correct and of high quality. In addition to identifying outliers, Q-Q plots are also used to assess data distributions. Multiple Q-Q plots are useful for performing point-by-point comparisons of grouped data sets, unlike box plots based upon the five-point summary statistics. ProUCL has Q-Q plots for normal, lognormal, and gamma distributions - not all of these graphical capabilities are directly available in other software packages such as NADA for R (Helsel 2013). ProUCL offers several exploratory options for generating Q-Q plots for data sets with NDs. Only detected outlying observations may require additional investigation; therefore, from an exploratory point of view, ProUCL can generate Q-Q plots excluding all NDs (and other options). Under this scenario there is no need to retain place holders (computing plotting positions used to impute NDs) as the objective is not to impute NDs. To impute NDs, ProUCL uses ROS methods (Gamma ROS and log ROS) requiring place holders; and ProUCL computes plotting positions for all detects and NDs to generate a proper regression model which is used to impute NDs. Also for comparison purposes, ProUCL can be used to generate Q-Q plots on data sets obtained by replacing NDs by their respective DLs or DL/2s. In these cases, no NDs are imputed, and there is no need to retain placeholders for NDs. On these Q-Q plots, ProUCL displays some relevant statistics which are computed based upon the data displayed on those graphs.

- Helsel (2012a) states that the **Summary Statistics** module does not display KM estimates and that statistics based upon logged data are useless. Typically, estimates computed after processing the data do not represent summary statistics. Therefore, KM and ROS estimates are not displayed in the **Summary Statistics** module. These statistics are available in several other modules including the UCL and BTV modules. At the request of several users, summary statistics are computed based upon logged data. It is believed that the mean, median, or standard deviation of logged data do provide useful information about data skewness and data variability.

- To test for the equality of variances, the F-test, as incorporated in ProUCL, performs fairly well and the inclusion of the Levene's (1960) test will not add any new capability to the ProUCL software. Therefore, taking budget constraints into consideration, Levene's test has not been incorporated in the ProUCL software.

    - Although it makes sense to first determine if the two variances are equal or unequal, this is not a requirement to perform a t-test. The t-distribution based confidence interval or test for μ_1 - μ_2 based on the pooled sample variance does not perform better than the approximate confidence intervals based upon Satterthwaite's test. Hence testing for the equality of variances is not required to perform a two-sample t-test. The use of Welch-Satterthwaite's or Cochran's method is recommended in all situations (see Hayes 2005).

- Helsel (2012a) suggests that imputed NDs should not be made available to the users. The developers of ProUCL and other researchers like to have access to imputed NDs. As a researcher, for exploratory purposes only, one may want to have access to imputed NDs to be used in exploratory advanced methods such as multivariate methods including data mining, cluster and principal component analyses. It is noted that one cannot easily perform exploratory methods on multivariate data sets with NDs. The availability of imputed NDs makes it possible for researchers and scientists to identify potential patterns present in complex multivariate data by using data mining exploratory methods on those multivariate data sets with NDs. Additional discussion on this topic is considered in Chapter 4 of the ProUCL 5.1 Technical Guide.

    - The statements summarized above should not be misinterpreted. One may not use parametric hypothesis tests such as a t-test or a classical ANOVA on data sets consisting of imputed NDs. These methods require further investigation as the decision errors associated with such methods remain unquantified. There are other methods such as the Gehan and T-W tests in ProUCL 5.0/ProUCL 5.1 which are better suited to perform two-sample hypothesis tests using data sets with multiple detection limits.

- Outliers: Helsel (2012a) and Helsel and Gilroy (2012) make several comments about outliers. The philosophy (with input from EPA scientists) of the developers of ProUCL about the outliers in environmental applications is that those outliers (unless they represent typographical errors) may potentially represent impacted (site related or otherwise) locations or monitoring wells; and therefore may require further investigation. Moreover, decision statistics such as a UCL95 based upon a data set with outliers gets inflated and tends to represent those outliers instead of representing the population average. Therefore, a few low probability outliers coming from the tails of the data distribution may not be included in the computation of the decision making upper limits (UCLs, UTLs), as those upper limits get distorted by outliers and tend not to represent the parameters they are supposed to estimate.

    - The presence of outliers in a data set tends to destroy the normality of the data set. In other words, a data set with outliers can seldom (may be when outliers are mild, lying around the border of the central and tail parts of a normal distribution) follow a normal distribution.

There are modern robust and resistant outlier identification methods (e.g., Rousseeuw and Leroy 1987; Singh and Nocerino 1995) which are better suited to identify outliers present in a data set; several of those robust outlier identification methods are available in the Scout 2008 version 1.0 (EPA 2009) software package.

- For both Rosner and Dixon tests, it is the data set (also called the main body of the data set) obtained after removing the outliers (and not the data set with outliers) that needs to follow a normal distribution (Barnett and Lewis 1994). Outliers are not known in advance. ProUCL has normal Q-Q plots which can be used to get an idea about potential outliers (or mixture populations) present in a data set. However, since a lognormal model tends to accommodate outliers, a data set with outliers can follow a lognormal distribution; this does not imply that the outlier which may actually represent an impacted/unusual location does not exist! In environmental applications, outlier tests should be performed on raw data sets, as the cleanup decisions need to be made based upon values in the raw scale and not in log-scale or some other transformed space. More discussion about outliers can be found in Chapter 7 of the ProUCL 5.1 Technical Guide.

- In Helsel (2012a), it is stated, "Mathematically, the lognormal is simpler and easier to interpret than the gamma (opinion)." We do agree with the opinion that the lognormal is simpler and easier to use but the log-transformation is often misunderstood and hence incorrectly used and interpreted. Numerous examples (e.g., Example 2-1 and 2-2, Chapter 2 of ProUCL Technical Guide) are provided in the ProUCL guidance documents illustrating the advantages of the using a gamma distribution.

- It is further stated in Helsel (2012a) that ProUCL prefers the gamma distribution because it downplays outliers as compared to the lognormal. This argument can be turned around - in other words, one can say that the lognormal is preferred by practitioners who want to inflate the effect of the outlier. Setting this argument aside, we prefer the gamma distribution as it does not transform the variable so the results are in the same scale as the collected data set. As mentioned earlier, log-transformation does appear to be simpler but problems arise when practitioners are not aware of the pitfalls (e.g., Singh and Ananda 2002; Singh, Singh, and Iaci 2002) associated with the use of lognormal distribution.

- Helsel (2012a) and Helsel and Gilroy (2012) state that "lognormal and gamma are similar, so usually if one is considered possible, so is the other." This is another incorrect and misleading statement; there are significant differences in the two distributions and in their mathematical properties. Based upon the extensive experience in environmental statistics and published literature, for skewed data sets that follow both lognormal and gamma distributions, the developers favor the use of the gamma distribution over the lognormal distribution. The use of the gamma distribution based decision statistics is preferred to estimate the environmental parameters (mean, upper percentile). A lognormal model tends to hide contamination by accommodating outliers and multiple populations whereas a gamma distribution tends not to accommodate contamination (elevated values) as can be seen in Examples 2-1 and 2-2 of Chapter 2 of the ProUCL 5.1 Technical Guide. The use of the lognormal distribution on a data set with outliers tends to yield inflated and distorted estimates which may not be protective of human health and the environment; this is especially true for skewed data sets of small of sizes <20-30; the sample size requirement increases with skewness.

    - In the context of computing a UCL95 of mean, Helsel and Gilroy (2012) and Helsel (2012a) state that GROS and LROS methods are probably never better than the KM method. It should be noted that these three estimation methods compute estimates of mean and standard deviation and not the upper limits used to estimate EPCs and BTVs. The use of the KM method does yield good estimates of the mean and standard deviation as noted by Singh, Maichle, and Lee (2006). The problem of estimating mean and standard deviation for data sets with nondetects has been studied by many researchers as described in Chapter 4 of the ProUCL 5.1 Technical Guide. Computing good estimates of mean and *sd* based upon left-censored data sets addresses only half of the problem. The main issue is to compute decision statistics (UCL, UPL, UTL) which account for uncertainty and data skewness inherently present in environmental data sets.

  - Realizing that for skewed data sets, Student's t-UCL, CLT-UCL, and standard and percentile bootstrap UCLs do not provide the specified coverage to the population mean for uncensored data sets, many researchers (e.g., Johnson 1978; Chen 1995; Efron and Tibshirani 1993; Hall [1988, 1992]; Grice and Bain 1980; Singh, Singh, and Engelhardt 1997; Singh, Singh, and Iaci 2002) developed parametric (e.g., gamma) and nonparametric (e.g., bootstrap-t and Hall's bootstrap method, modified-t, and Chebyshev inequality) methods for computing confidence intervals and upper limits which adjust for data skewness. One cannot ignore the work and findings of the researchers cited above, and assume that Student's t-statistic based upper limits or percentile bootstrap method based upper limits can be used for all data sets with varying skewness and sample sizes.

  - Analytically, it is not feasible to compare the various estimation and UCL computation methods for skewed data sets containing ND observations. Instead, researchers use simulation experiments to learn about the distributions and performances of the various statistics (e.g., KM-t-UCL, KM-percentile bootstrap UCL, KM-bootstrap-t UCL, KM-Gamma UCL). Based upon the suggestions made in published literature and findings summarized in Singh, Maichle, and Lee (2006), it is reasonable to state and assume that the findings of the simulation studies performed on uncensored skewed data sets comparing the performances of the various UCL computation methods can be extended to skewed left-censored data sets.

  - Like uncensored skewed data sets, for left-censored data sets, ProUCL 5.0/ProUCL 5.1 has several parametric and nonparametric methods to compute UCLs and other limits which adjust for data skewness. Specifically, ProUCL uses KM estimates in gamma equations; in the bootstrap-t method, and in the Chebyshev inequality to compute upper limits for left-censored skewed data sets.

- Helsel (2012a) states that ProUCL 4 is based upon presuppositions. It is emphasized that ProUCL does not make any suppositions in advance. Due to the poor performance of a lognormal model, as demonstrated in the literature and illustrated via examples throughout ProUCL guidance documents, the use of a gamma distribution is preferred when a data set can be modeled by a lognormal model and a gamma model. To provide the desired coverage (as close as possible) for the population mean, in earlier versions of ProUCL (version 3.0), in lieu of H-UCL, the use of Chebyshev UCL was suggested for moderately and highly skewed data sets. In later (3.00.02 and higher) versions of ProUCL, depending upon skewness and sample size, for gamma distributed data sets, the use of the gamma distribution was suggested for computing the UCL of the mean.

Upper limits (e.g., UCLs, UPLs, UTLs) computed using the Student's t statistic and percentile bootstrap method (Helsel 2012, NADA for R, 2013) often fail to provide the desired coverage (e.g., 95% confidence coefficient) to the parameters (mean, percentile) of most of the skewed environmental populations. It is suggested that the practitioners compute the decision making statistics (e.g., UCLs, UTLs) by taking: data *distribution; data set size; and data skewness into consideration. For uncensored and left-censored data sets, several such upper limits computation methods are available in ProUCL 5.1 and its earlier versions.*

Contrary to the statements made in Helsel and Gilroy (2012), ProUCL software does not favor statistics which yield higher (e.g., nonparametric Chebyshev UCL) or lower (e.g., preferring the use of a gamma distribution to using a lognormal distribution) estimates of the environmental parameters (e.g., EPC and BTVs). The main objectives of the ProUCL software funded by the U.S. EPA is to compute rigorous decision statistics to help the decision makers and project teams in making sound decisions which are cost-effective and protective of human health and the environment.

Cautionary Note: Practitioners and scientists are cautioned about: 1) the suggestions made about the computations of upper limits described in some recent environmental literature such as the NADA books (Helsel [2005, 2012]); and 2) the misleading comments made about the ProUCL software in the training courses offered by Practical Stats during 2012 and 2013. Unfortunately, comments about ProUCL made by Practical Stats during their training courses lack professionalism and theoretical accuracy. It is noted that NADA packages in R and Minitab (2013) developed by Practical Stats do not offer methods which can be used to compute reliable or accurate decision statistics for skewed data sets. Decision statistics (e.g., UCLs, UTLs, UPLs) computed using the methods (e.g., UCLs computed using percentile bootstrap, and KM and LROS estimates and t-critical values) described in the NADA books and incorporated in NADA packages do not take data distribution and data skewness into consideration. The use of statistics suggested in NADA books and in Practical Stats training sessions often fail to provide the desired specified coverage to environmental parameters of interest for moderately skewed to highly skewed populations. Conclusions derived based upon those statistics may lead to incorrect conclusions which may not be cost-effective or protective of human health and the environment.

Page 75 (Helsel [2012]): One of the reviewers of the ProUCL 5.0 software drew our attention to the following incorrect statement made on page 75 of Helsel (2012):

"If there is only 1 reporting limit, the result is that the mean is identical to a substitution of the reporting limit for censored observations."

An example of a left-censored data set containing ND observations with one reporting limit of 20 which illustrates this issue is described as follows.

Y	D_y
20	0
20	0
20	0
7	1
58	1
92	1
100	1
72	1
11	1
27	1

The mean and standard deviation based upon the KM and two substitution methods: DL/2 and DL are summarized as follows:

Kaplan-Meier (KM) Statistics
Mean 39.4
SD 35.56

DL Substitution method (replacing censored values by the reporting limit)
Mean 42.7
SD 34.77

DL/2 Substitution method (replacing NDs by the reporting limit)
Mean 39.7
SD 37.19

The above example illustrates that the KM mean (when only 1 detection limit is present) is not actually identical to the mean estimate obtained using the substitution, DL (RL) method. The statement made in Helsel's text (and also incorrectly made in his presentations such as the one made at the U.S. EPA 2007 National Association of Regional Project Managers (NARPM) Annual Conference: http://www.ttemidev.com/narpm2007Admin/conference/) holds only when all observations reported as detects are greater than the single reporting limit, which is not always true for environmental data sets consisting of analytical concentrations.

1.16 Box and Whisker Plots

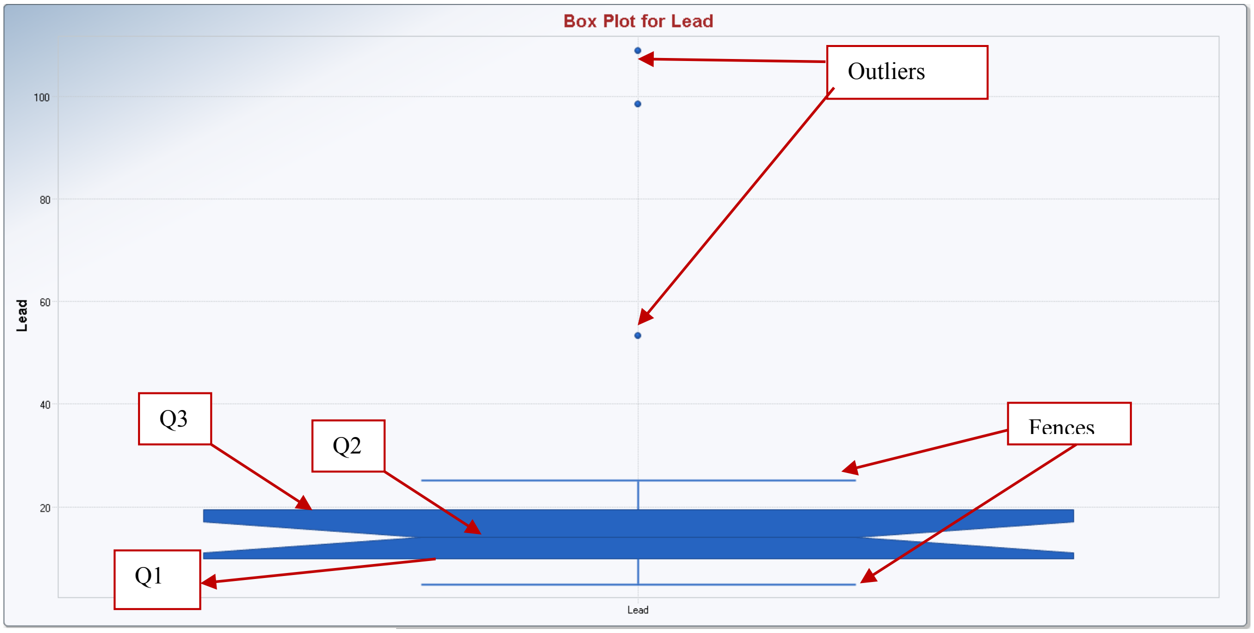
At the request of ProUCL users, a brief description of box plots (also known as box and whisker plots) as developed by Tukey (Hoaglin, Mosteller and Tukey 1991) is provided in this section. A box and whiskers plot represents a useful and convenient *exploratory* tool and provides a quick five-point summary of a data set. In statistical literature, one can find several ways to generate box plots. The practitioners may have their own preferences to use one method over the other. Box plots are well documented in the statistical literature and description of box plots can be easily obtained by surfing the net. Therefore, the detailed description about the generation of box plots is not provided in ProUCL guidance documents. ProUCL also generates box plots for data set with NDs. Since box plots are used for exploratory purposes to identify outliers and also to compare concentrations of two or more groups, it does not really matter how NDs are displayed on those box plots. ProUCL generates box plots using detection limits and draws a horizontal line at the highest detection limit. Users can draw up to four horizontal lines at other levels (e.g., a screening level, a BTV, or an average) of their choice.

All box plot methods, including the one in ProUCL, represent five-point summary graphs including: the lowest and the highest data values, median (50^{th} percentile=second quartile, Q2), 25^{th} percentile (lower quartile, Q1), and 75^{th} percentile (upper quartile, Q3). A box and whisker plot also provides information about the degree of dispersion (interquartile range (IQR) = Q3-Q1=length/height of the box in a box plot), the degree of skewness (suggested by the length of the whiskers) and unusual data values known as outliers. Specifically, ProUCL (and other software packages) use the following to generate a box and whisker plot.

- Q1= 25^{th} percentile, Q2= 50^{th} (median), and Q3 = 75^{th} percentile
- Interquartile range= IQR = Q3-Q1 (the length/height of the box in a box plot)
- Lower whisker starts at Q1 and the upper whisker starts at Q3.
- Lower whisker extends up to the lowest observation or (Q1 - 1.5 * IQR) whichever is higher
- Upper whisker extends up to the highest observation or (Q3 + 1.5 * IQR) whichever is lower

- Horizontal bars (also known as fences) are drawn at the end of whiskers
- Guidance in statistical literature suggests that observations lying outside the fences (above the upper bar and below the lower bar) are considered potential outliers

An example box plot generated by ProUCL is shown in the following graph.



Box Plot with Fences and Outlier

It should be pointed out that the use of box plots in different scales (e.g., raw-scale and log-scale) may lead to different conclusions about outliers. Below is an example illustrating this issue.

Example 1-2. Consider an actual data set consisting of copper concentrations collected a Superfund Site. The data set is: 0.83, 0.87, 0.9, 1, 1, 2, 2, 2.18, 2.73, 5, 7, 15, 22, 46, 87.6, 92.2, 740, and 2960. Box plots using data in the raw-scale and log-scale are shown in Figures 1-1 and 1-2.

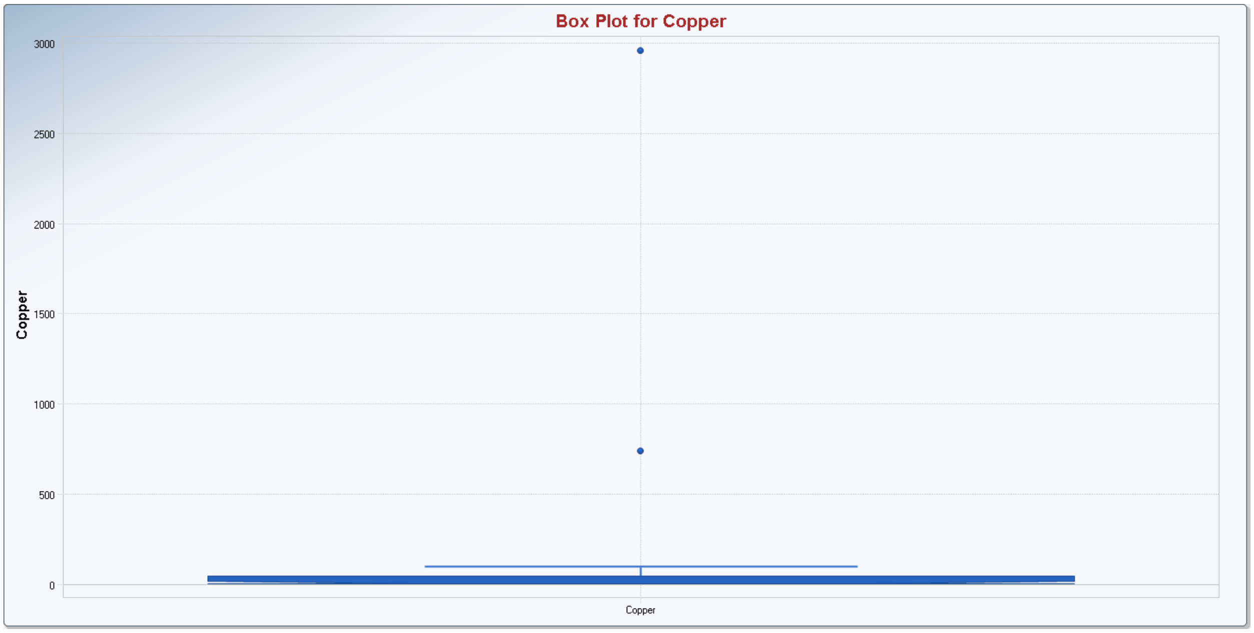


Figure 1-1. Box Plot of Raw Data in Original Scale

Based upon the last bullet point of the description of box plots described above, from Figure 1-1, it is concluded that two observations 740 and 2960 in the raw scale represent outliers.

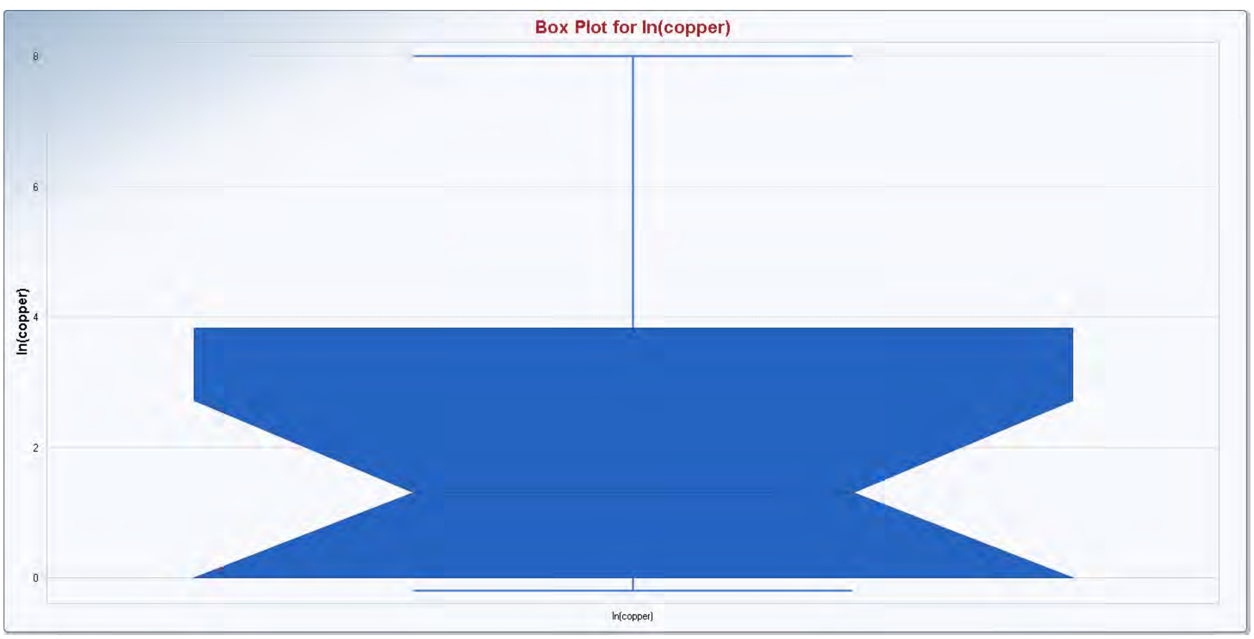


Figure 1-2. Box Plot of Data in Log-Scale

However, based upon the last bullet point about box plots, from Figure 1-2, it is concluded that two observations 740 and 2960 in the log-scale do not represent outliers. The log-transformation has accommodated the two outliers. This is one of the reasons ProUCL guidance suggests avoiding the use of log-transformed data. The use of a log-transformation tends to hide/accommodate outliers/contamination.

Note: ProUCL uses a couple of development tools such as FarPoint spread (for Excel type input and output operations) and ChartFx (for graphical displays). ProUCL generates box plots using the built-in box plot feature in ChartFx. The programmer has no control over computing various statistics (e.g., Q1, Q2, Q3, IQR) using ChartFx. So box plots generated by ProUCL can differ slightly from box plots generated by other programs (e.g., Excel). However, for all practical and exploratory purposes, box plots in ProUCL are equally good (if not better) as available in the various commercial software packages for investigating data distribution (skewed or symmetric), identifying outliers, and comparing multiple groups (main objectives of box plots).

Precision in Box Plots: Box plots generated using ChartFx round values to the nearest integer. For increased precision of graphical displays (all graphical displays generated by ProUCL), the user can use the process described as follows.

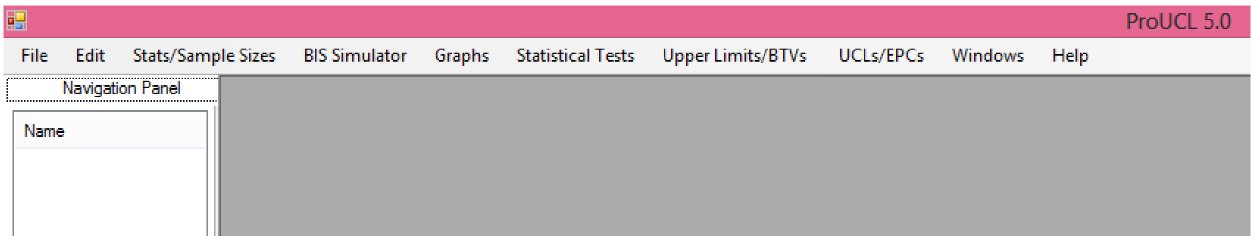
Position your cursor on the graph and right-click, a popup menu will appear. Position the cursor on **Properties** and right-click; a windows form labeled **Properties** will appear. There are three choice at the top: **General**, **Series** and **Y-Axis**. Position the e cursor over the **Y-Axis** choice and left-click. You can change the number of decimals to increase the precision, change the step to increase or decrease the number Y-Axis values displayed and/or change the direction of the label. To show values on the plot itself, position your cursor on the graph and right-click; a pop-up menu will appear. Position the cursor on **Point Labels** and right-click. There are other options available in this pop-up menu including changing font sizes.

Chapter 2

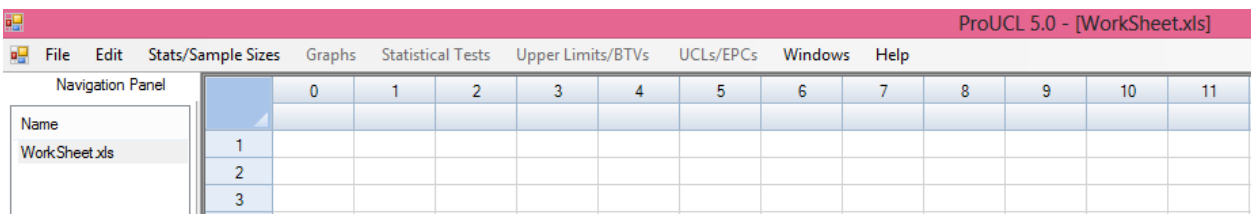
Entering and Manipulating Data

2.1 Creating a New Data Set

By executing ProUCL 5.1, the following file options will appear (the title will show ProUCL 5.1 instead of ProUCL 5.0):

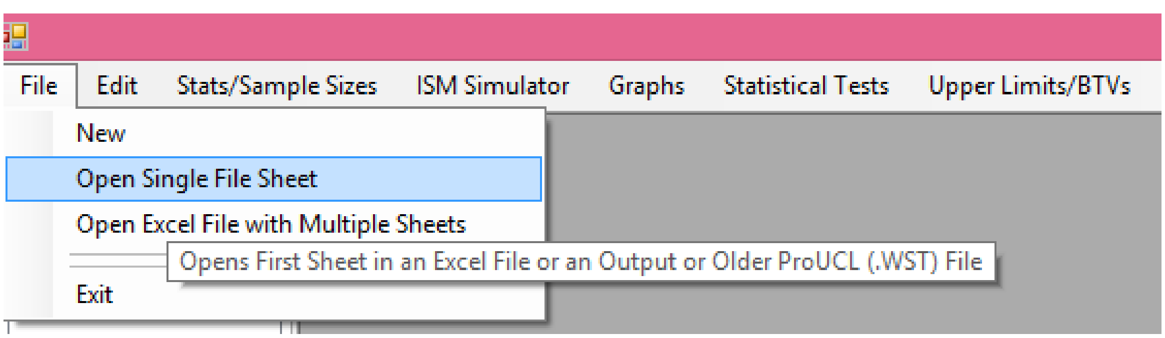


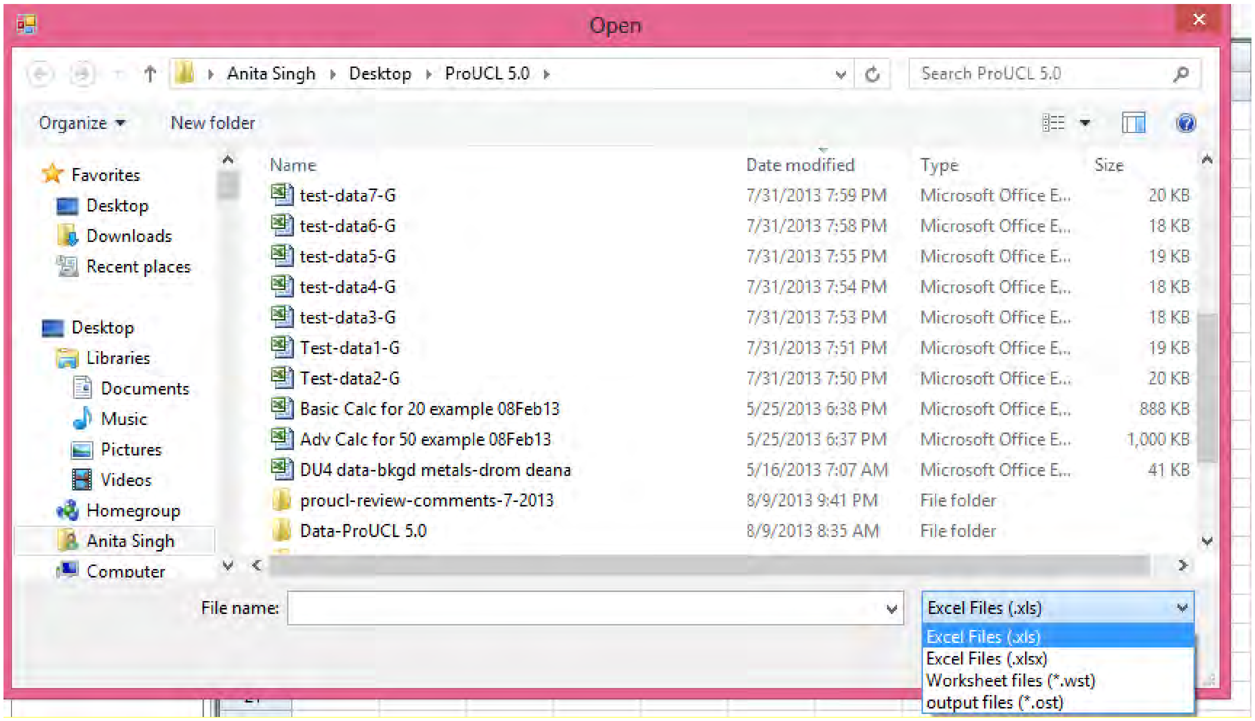
By choosing the **File ► New** option, a new worksheet shown below will appear. The user enters variable names and data following the ProUCL input file format requirements described in Section 2.3.



2.2 Opening an Existing Data Set

The user can open an existing worksheet (*.xls, *.xlsx, *.wst, and *.ost) by choosing the **File ► Open Single File Sheet** option. The following drop down menu will appear:





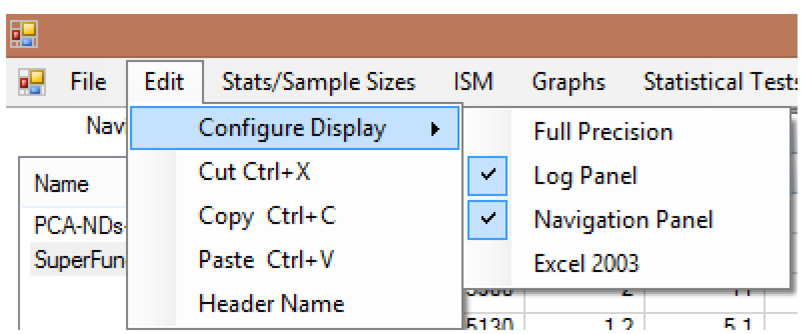
Choose a file by high lighting the type of file such as **.xls** as shown above. This option can also be used to read in a *.wst worksheet and *.ost output sheet generated by earlier versions (e.g., ProUCL 4.1 and older) of ProUCL.

By choosing the **File ► Excel Multiple Sheets** option, the user can open an Excel file consisting of multiple sheets. Each sheet will be opened as a separate file to be processed individually by ProUCL 5.1

Caution: If you are editing a file (e.g., an excel file using Excel), make sure to close the file before importing the file into ProUCL using the file open option.

2.3 Input File Format

- The program can read Excel files. The user can perform typical Cut, Paste, and Copy operations available under the Edit Menu Option as shown below.



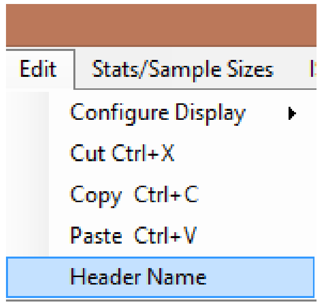
- The first row in all input data files consist of alphanumeric (strings of numbers and characters) names representing the header row. Those header names may represent meaningful variable names such as Arsenic, Chromium, Lead, Group-ID, and so on.
    - The Group-ID column holds the labels for the groups (e.g., Background, AOC1, AOC2, 1, 2, 3, a, b, c, Site 1, Site 2) that might be present in the data set. Alphanumeric strings (e.g., Surface, Sub-surface) can be used to label the various groups. Most of the modules of ProUCL can process data by a group variable.
    - The data file can have multiple variables (columns) with unequal numbers of observations. Most of the modules of ProUCL can process data by a group variable.
    - Except for the header row and columns representing the group labels, only numerical values should appear in all other rows.
    - All alphanumeric strings and characters (e.g., blank, other characters, and strings), and all other values (that do not meet the requirements above) in the data file are treated as missing values and are omitted from statistical evaluations.
    - Also, a large value denoted by 1E31 (= 1×10^{31}) can be used to represent missing data values. All entries with this value are ignored from the computations. These values are counted under the number of missing values.

2.4 Number Precision

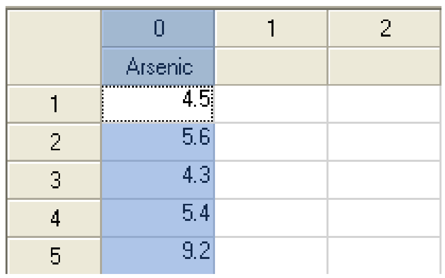
- The user may turn "Full Precision" on or off by choosing **Configure ► Full Precision On/OFF**
- By leaving "Full Precision" turned **off**, ProUCL will display numerical values using an appropriate (default) decimal digit option; and by turning "Full Precision" **off**, all decimal values will be rounded to the nearest thousandths place.
- The "Full Precision" **on** option is specifically useful when dealing with data sets consisting of small numerical values (e.g., < 1) resulting in small values of the various estimates and test statistics. These values may become so small with several leading zeros (e.g., 0.00007332) after the decimal. In such situations, one may want to use the "Full Precision" **on** option to see nonzero values after the decimal.

*<u>Note:</u> For the purpose of this User Guide, unless noted otherwise, all examples have used the "Full Precision" **OFF** option. This option prints out results up to 3 significant digits after the decimal.*

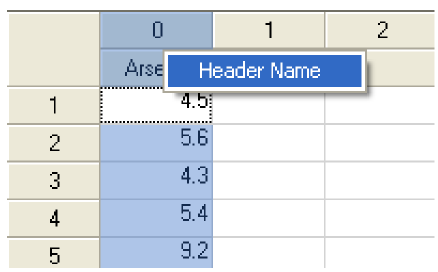
2.5 Entering and Changing a Header Name



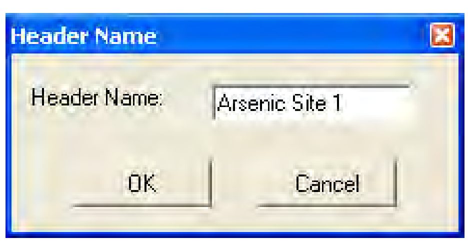
1. The user can change variable names (Header Name) using the following process. Highlight the column whose header name (variable name) you want to change by clicking either the column number or the header as shown below.



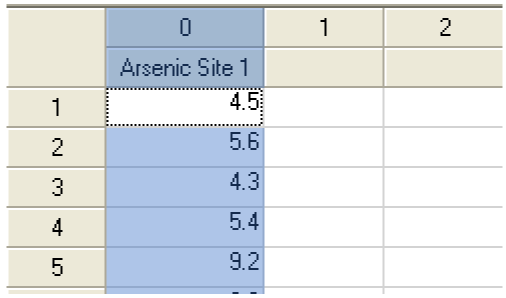
2. Right-click and then click **Header Name**.



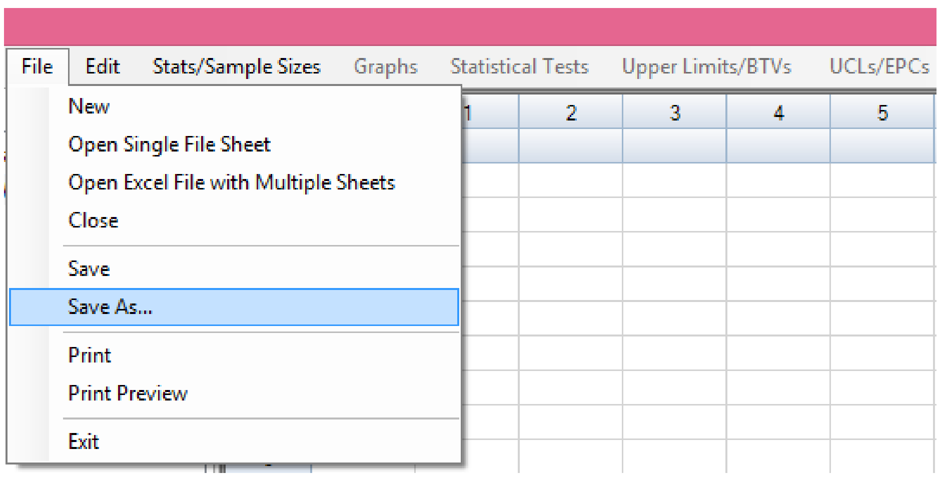
3. Change the Header Name.



4. Click the **OK** button to get the following output with the changed variable name.



2.6 Saving Files

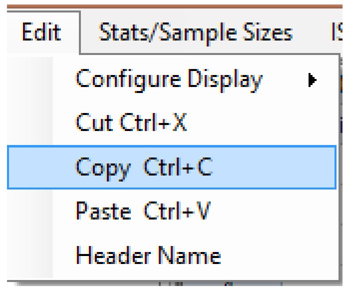


- The **Save** option allows the user to save the active window in Excel 2003 or Excel 2007.

  The **Save As** option also allows the user to save the active window. This option follows typical Windows standards, and saves the active window to a file in .xls or .xlsx format. All modified/edited data files, and output screens (excluding graphical displays) generated by the software can be saved as .xls or .xlsx files.

2.7 Editing

Click on the Edit menu item to reveal the following drop-down options.



- **Cut** option: similar to a standard Windows Edit option, such as in Excel. It performs standard edit functions on selected highlighted data (similar to a buffer).

- **Copy** option: similar to a standard Windows Edit option, such as in Excel. It performs typical edit functions on selected highlighted data (similar to a buffer).

  Paste option: similar to a standard Windows Edit option, such as in Excel. It performs typical edit functions of pasting the selected (highlighted) data to the designated spreadsheet cells or area.

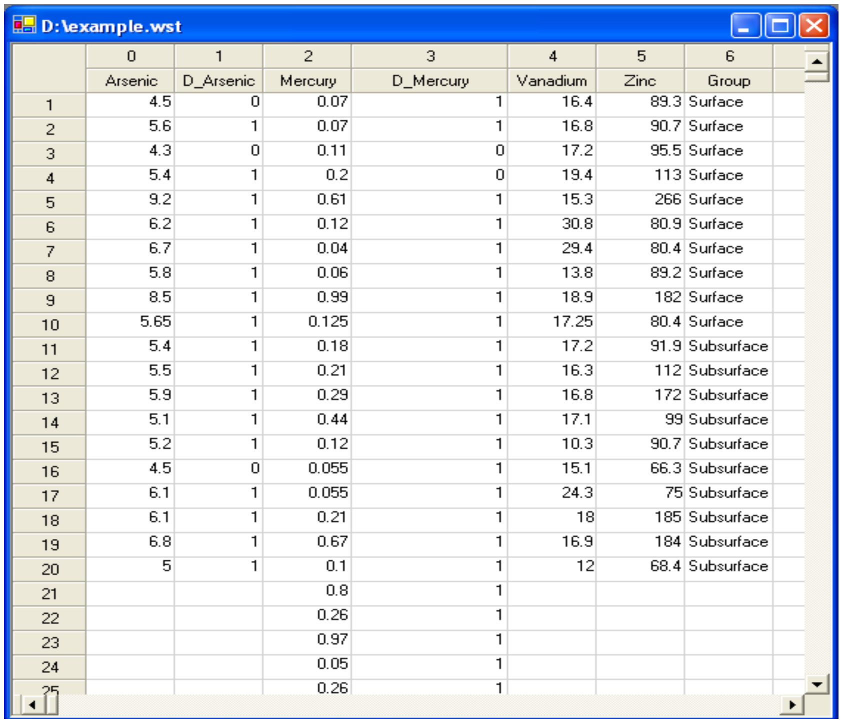
2.8 Handling Nondetect Observations and Generating Files with Nondetects

- Several modules of ProUCL (e.g., Statistical Tests, Upper limits/BTVs, UCLs/EPCs) handle data sets containing ND observations with single and multiple DLs.

- The user informs the program about the status of a variable consisting of NDs. For a variable with ND observations (e.g., arsenic), the detected values, and the numerical values of the associated detection limits (for less than values) are entered in the appropriate column associated with that variable. No qualifiers or flags (e.g., J, B, U, UJ, X) should be entered in data files with ND observations.

- Data for variables with ND values are provided in two columns. One column consists of numerical values of detected observations and numerical values of detection limits (or reporting limits) associated with observations reported as NDs; and the second column represents their detection status consisting of only 0 (for ND values) and 1 (for detected values) values. The name of the corresponding variable representing the detection status should start with d_, or D_ (not case sensitive) and the variable name. The detection status column with variable name starting with a D_ (or a d_) should have only two values: 0 for ND values, and 1 for detected observations.

- For example, the header name, D_Arsenic is used for the variable, Arsenic having ND observations. The variable D_Arsenic contains a 1 if the corresponding Arsenic value represents a detected entry, and contains a 0 if the corresponding entry represents a ND entry. If this format is not followed, the program will not recognize that the data set has NDs. An example data set illustrating these points is given as follows. ProUCL does not distinguish between lowercase and uppercase letters.



D:\example.wst

	0	1	2	3	4	5	6
	Arsenic	D_Arsenic	Mercury	D_Mercury	Vanadium	Zinc	Group
1	4.5	0	0.07	1	16.4	89.3	Surface
2	5.6	1	0.07	1	16.8	90.7	Surface
3	4.3	0	0.11	0	17.2	95.5	Surface
4	5.4	1	0.2	0	19.4	113	Surface
5	9.2	1	0.61	1	15.3	266	Surface
6	6.2	1	0.12	1	30.8	80.9	Surface
7	6.7	1	0.04	1	29.4	80.4	Surface
8	5.8	1	0.06	1	13.8	89.2	Surface
9	8.5	1	0.99	1	18.9	182	Surface
10	5.65	1	0.125	1	17.25	80.4	Surface
11	5.4	1	0.18	1	17.2	91.9	Subsurface
12	5.5	1	0.21	1	16.3	112	Subsurface
13	5.9	1	0.29	1	16.8	172	Subsurface
14	5.1	1	0.44	1	17.1	99	Subsurface
15	5.2	1	0.12	1	10.3	90.7	Subsurface
16	4.5	0	0.055	1	15.1	66.3	Subsurface
17	6.1	1	0.055	1	24.3	75	Subsurface
18	6.1	1	0.21	1	18	185	Subsurface
19	6.8	1	0.67	1	16.9	184	Subsurface
20	5	1	0.1	1	12	68.4	Subsurface
21			0.8	1			
22			0.26	1			
23			0.97	1			
24			0.05	1			
25			0.26	1			

2.9 Caution

- Care should be taken to avoid any misrepresentation of detected and nondetected values. Specifically, do not include any missing values (blanks, characters) in the D_column (detection status column). If a missing value is located in the D_column (and not in the associated variable column), the corresponding value in the variable column is treated as a ND, even if this might not have been the intention of the user.

- It is mandatory that the user makes sure that only a 1 or a 0 are entered in the detection status D_column. If a value other than a 0 or a 1 (such as qualifiers) is entered in the D_ column (the detection column), results may become unreliable, as the software defaults to any number other than 0 or 1 as a ND value.

- When computing statistics for full uncensored data sets without any ND values, the user should select only those variables (from the list of available variables) that contain no ND observations. Specifically, ND values found in a column chosen for the summary statistics (full-uncensored data set) will be treated as a detected value; whatever value (e.g., detection limit) is entered in that column will be used to compute summary statistics for a full-uncensored data set without any ND values.

- It is mandatory that the header name of a nondetect column associated with a variable such as XYZ should be D_XYZ (or d_Xyz). No other characters or blanks are allowed. However, the header (column) names are not case sensitive. If the nondetect column is not labeled properly, methods to handle nondetect data will not be activated and shown.

- **Two-Sample Hypotheses:** When using two-sample hypotheses tests (WMW test, Gehan test, and T-W test) on data sets with NDs, both samples or variables (e.g., site-As, Back-As) should be specified as having NDs, even though one of the variables may not have any ND observations. This means that a ND column (with 0 = ND, and 1 = detect) should be provided for each variable (here D_site-As, and D_Back-As) to be used in this comparison. *If a variable (e.g., site-As) does not have any NDs, still a column with label D_site-As should be included in the data set with all entries = 1 (detected values).*

- The sample data set given on the previous page illustrates points related to this option and issues listed above. The data set contains some ND measurements for arsenic and mercury. It should be noted that mercury concentrations are used to illustrate the points related to ND observations; arsenic and zinc concentrations are used to illustrate the use of the group variable, Group (Surface, Subsurface).

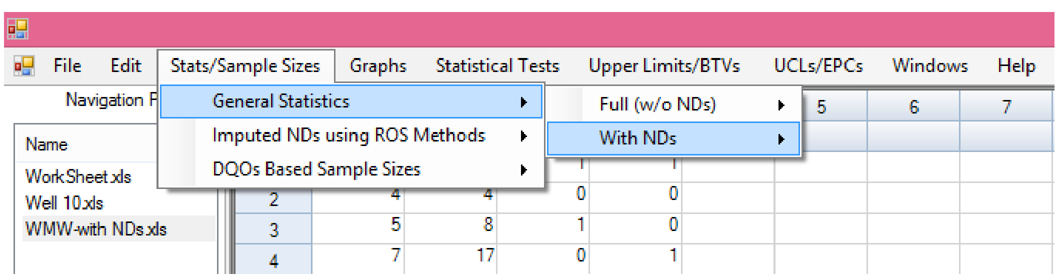
- If for mercury, one computes summary statistics (assuming no ND values) using "Full" data set option, then all ND values (with "0" entries in D_Mercury column) will be treated as detected values, and summary statistics will be computed accordingly.

2.10 Summary Statistics for Data Sets with Nondetect Observations

- To compute statistics of interest (e.g., background statistics, GOF test, UCLs, WMW test) for variables with ND values, one should choose the ND option, **With NDs**, from the available menu options such as **Stats/Sample Sizes**, **Graphs**, **Statistical Tests**, **Upper Limits/BTVs**, and **UCLs/EPCs**.

- The NDs option of these modules gets activated only when your data set contains NDs.

- For data sets with NDs, the **Stats/Sample Sizes** module of ProUCL 5.0 computes summary statistics and other general statistics such as the KM mean and KM standard deviation based upon raw as well as log-transformed data.



- The **General Statistics/With NDs** option also provides simple statistics (e.g., % NDs, Max detect, Min detect, Mean) based upon detected values. The statistics computed in log-scale (e.g., *sd* of log-transformed detected values) may help a user to determine the degree of skewness (e.g., mild, moderate, high) of a data set based upon detected values. These statistics may also help the user to choose the most appropriate method (e.g., KM bootstrap-t UCL or KM percentile bootstrap UCL) to compute UCLs, UPLs, and other limits used to compute decision statistics.

- All other parametric and nonparametric statistics and estimates of population mean, variance, percentiles (e.g., KM, and ROS estimates) for variables with ND observations are provided in other menu options such as **Upper Limits/BTVs** and **UCLs/EPCs**.

2.11 Warning Messages and Recommendations for Data Sets with an Insufficient Amount of Data

- ProUCL provides warning messages and recommendations for data sets with an insufficient amount of data for calculating meaningful estimates and statistics of interest. For example, it is not desirable to compute an estimate of the EPC term based upon a discrete (as opposed to composite or ISM) data set of size less than 5, especially when NDs are also present in the data set.

- However, to accommodate the computation of UCLs and other limits based upon ISM data sets, ProUCL 5.0 allows users to compute UCLs, UPLs, and UTLs based upon data sets of sizes as small as 3. The user is advised to follow the guidance provided in the ITRC ISM Technical Regulatory Guidance Document (2012) to select an appropriate UCL95 to estimate the EPC term. Due to lower variability in ISM data, the minimum sample size requirements for statistical methods used on ISM data are lower than the minimum sample size requirements for statistical methods used on discrete data sets.

- It is suggested that for data sets composed of observations resulting from discrete sampling, at least 10 observations should be collected to compute UCLs and various other limits.

- Some examples of data sets with insufficient amount of data include data sets with less than 3 distinct observations, data sets with only one detected observation, and data sets consisting of all nondetects.

- Some of the warning messages generated by ProUCL 5.0 are shown as follows.

UCL Statistics for Uncensored Full Data Sets

User Selected Options	
Date/Time of Computation	3/13/2013 9:26:43 PM
From File	Not-enough-data-set.xls
Full Precision	OFF
Confidence Coefficient	95%
Number of Bootstrap Operations	2000

x

General Statistics

Total Number of Observations	2	Number of Distinct Observations	2
		Number of Missing Observations	0
Minimum	2	Mean	4.5
Maximum	7	Median	4.5

Warning: This data set only has 2 observations!
Data set is too small to compute reliable and meaningful statistics and estimates!
The data set for variable x was not processed!

It is suggested to collect at least 8 to 10 observations before using these statistical methods!
If possible, compute and collect Data Quality Objectives (DQO) based sample size and analytical results.

UCL Statistics for Data Sets with Non-Detects	
User Selected Options	
Date/Time of Computation	3/13/2013 9:27:39 PM
From File	Not-enough-data-set.xls
Full Precision	OFF
Confidence Coefficient	95%
Number of Bootstrap Operations	2000

y

General Statistics			
Total Number of Observations	7	Number of Distinct Observations	6
Number of Detects	2	Number of Non-Detects	5
Number of Distinct Detects	2	Number of Distinct Non-Detects	4
Minimum Detect	10	Minimum Non-Detect	1
Maximum Detect	13	Maximum Non-Detect	5
Variance Detects	4.5	Percent Non-Detects	71.43%
Mean Detects	11.5	SD Detects	2.121
Median Detects	11.5	CV Detects	0.184
Skewness Detects	N/A	Kurtosis Detects	N/A
Mean of Logged Detects	2.434	SD of Logged Detects	0.186

Warning: Data set has only 2 Detected Values.
This is not enough to compute meaningful or reliable statistics and estimates.

Normal GOF Test on Detects Only

Not Enough Data to Perform GOF Test

	Background Statistics for Data Sets with Non-Detects
User Selected Options	
From File	Not-enough-data-set_a.xls
Full Precision	OFF
Confidence Coefficient	95%
Coverage	95%
Different or Future K Observations	1
Number of Bootstrap Operations	2000

yy

General Statistics			
Total Number of Observations	7	Number of Missing Observations	0
Number of Distinct Observations	6		
Number of Detects	0	Number of Non-Detects	7
Number of Distinct Detects	0	Number of Distinct Non-Detects	6
Minimum Detect	N/A	Minimum Non-Detect	1
Maximum Detect	N/A	Maximum Non-Detect	13
Variance Detected	N/A	Percent Non-Detects	100%
Mean Detected	N/A	SD Detected	N/A
Mean of Detected Logged Data	N/A	SD of Detected Logged Data	N/A

Warning: All observations are Non-Detects (NDs), therefore all statistics and estimates should also be NDs!
Specifically, sample mean, UCLs, UPLs, and other statistics are also NDs lying below the largest detection limit!
The Project Team may decide to use alternative site specific values to estimate environmental parameters (e.g., EPC, BTV).

The data set for variable yy was not processed!

2.12 Handling Missing Values

- The modules (e.g., Stats, GOF, UCLs, BTVs, Regression, Trend tests) of ProUCL 5.0 can handle missing values within a data set. Appropriate messages are displayed when deemed necessary.

- All blanks, alphanumeric strings (except for group variables), or the specific large value 1e31 are considered as missing values.

- A group variable (representing two or more groups, populations, MWs) can have alphanumeric values (e.g., MW01, MW02, AOC1, AOC2).

- ProUCL ignores all missing values in all statistical evaluations it performs. Missing values are therefore not treated as being part of a data set.

- Number of Valid Samples or Number of Valid Observations represents the Total Number of Observations minus the Number of Missing Values. If there are no missing values, then number of valid samples = total number of observations.

  Valid Samples = Total Number of Observations – Missing Values.

- It is important to note, however, that if a missing value not meant (e.g., a blank, or 1e31) to represent a group category is present in a "Group" variable, ProUCL 5.1/ProUCL 5.0 will treat that blank value (or 1e31 value) as a new group. All variables and values that correspond to this missing value will be treated as part of a new group and not with any existing groups. It is therefore important to check the consistency and validity of all data sets before performing statistical evaluations.

- ProUCL prints out the number of missing values (if any) and the number of reported values (excluding the missing values) associated with each variable in the data sheet. This information is provided in several output sheets (e.g., General statistics, BTVs, UCLs, Outliers, OLS, Trend Tests) generated by ProUCL 5.1.

- Number of missing values in Regression: The OLS module also handles the number of missing values in the two columns (X and Y) representing independent (X) and dependent (Y) variables. ProUCL provides warning messages for bad data sets (e.g., all identical values) when statistics of interest cannot be computed. However, a bad/extreme data set can occur in numerous different ways, and ProUCL may not cover all of those extreme/bad data sets. In such cases, ProUCL may still yield an error message. The user needs to review and fix his data set before performing regression or trend analysis again.

For further clarification of labeling missing values, the following example illustrates the terminology used for the number of valid samples and of unique and distinct samples on output sheets generated by the ProUCL software.

Example: The following example illustrates the notion of Valid Samples, Unique or Distinct Samples, and Missing Values. The data set also has ND values. ProUCL 5.0 computes these numbers and prints them on the UCLs and background statistics output.

x	D_x
2	1
4	1
2.3	1
1.2	0
w34	0
1.0E+031	0
	0
anm	0
34	1
23	1
0.5	0
0.5	0
2.3	1
2.3	1
2.3	1
34	1
73	1

Valid Samples: Represents the total number of observations (censored and uncensored inclusive) excluding the missing values. In this case the number of valid samples = 9. If a data set has no missing value, then the total number of data points equals number of valid samples.

Missing Values: All values not representing a real numerical number are treated as missing values. Specifically, all alphanumeric values including blanks are considered to be missing values. Big numbers such as 1.0e31 are also treated as missing values and are considered as not valid observations. In the example above the number of missing values = 4.

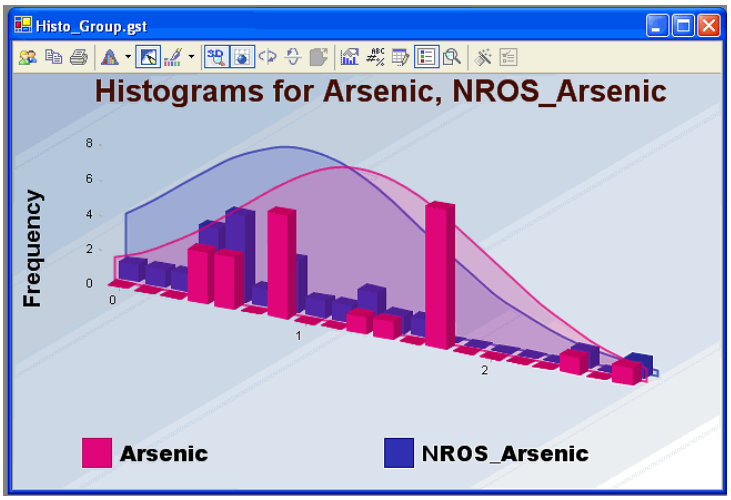
Unique or Distinct Samples: The number of unique samples or number of distinct samples represents all unique (or distinct) detected and nondetected values. This is computed separately for detects and NDs. This number is especially useful when using bootstrap methods. As well known, it is not desirable and advisable to use bootstrap methods, when the number of unique samples is small. In the example above total number of unique or distinct samples = 8, number of distinct detects = 6, and number of distinct NDs (with different detection limits) = 2.

x			
	General Statistics		
Total Number of Observations	13	Number of Distinct Observations	8
		Number of Missing Observations	4
Number of Detects	10	Number of Non-Detects	3
Number of Distinct Detects	6	Number of Distinct Non-Detects	2
Minimum Detect	2	Minimum Non-Detect	0.5
Maximum Detect	73	Maximum Non-Detect	1.2
Variance Detects	555.5	Percent Non-Detects	23.08%

2.13 User Graphic Display Modification

Advanced users are provided two sets of tools to modify graphics displays. A graphics tool bar is available above the graphics display; the user can right-click on the desired object within the graphics display, and a drop-down menu will appear. The user can select an item from the drop-down menu list by clicking on that item. This will allow the user to make modifications as available for the selected menu item. An illustration is given as follows.

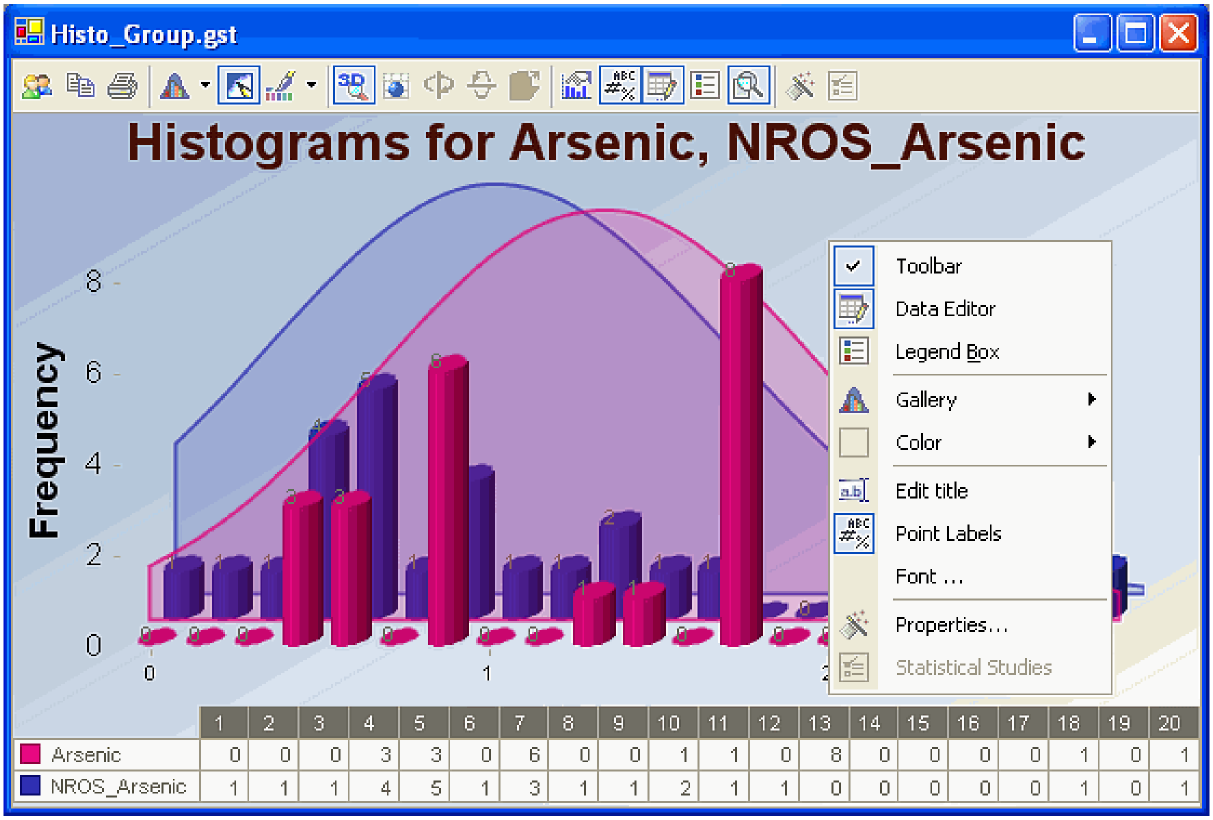
2.13.1 Graphics Tool Bar

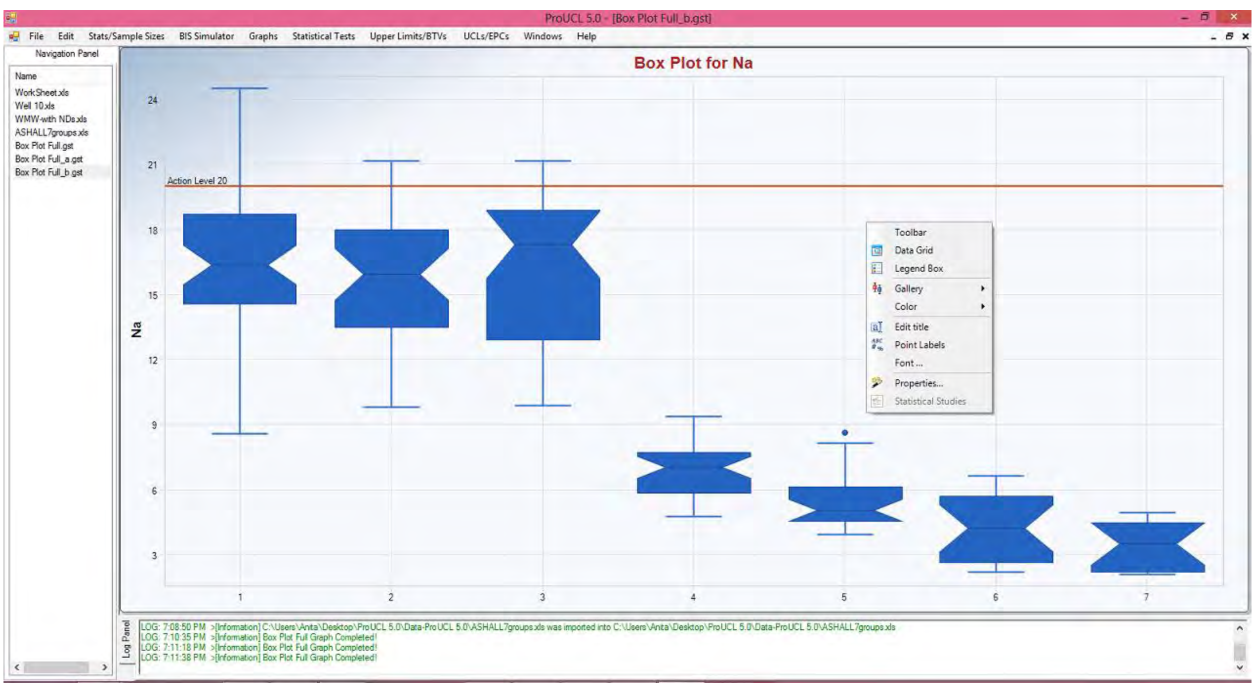


The user can change fonts, font sizes, vertical and horizontal axis's, select new colors for the various features and text. All these actions are generally used to modify the appearance of the graphic display. The user is cautioned that these tools can be unforgiving and may put the user in a situation where the user cannot go back to the original display. Users are on their own in exploring the robustness of these tools. Therefore, less experienced users may not want to use these drop-down menu graphic tools.

2.13.2 Drop-Down Menu Graphics Tools

Graphs can be modified by using the options shown on the two graphs displayed below. These tools allow the user to move the mouse to a specific graphic item like an axis label or a display feature. The user then right-clicks their mouse and a drop-down menu will appear. This menu presents the user with available options for that particular control or graphic object. For example, the user can change colors, title name, axes labels, font size, and re-size the graphs. There is less chance of making an unrecoverable error but that risk is always present. As a cautionary note, the user can always delete the graphics window and redraw the graphical displays by repeating their operations from the datasheet and menu options available in ProUCL. A couple of examples of a drop-down menu obtained by right-clicking the mouse on the background area of the graphics display are given as follows.


Histo_Group.gst
Histograms for Arsenic, NROS_Arsenic
Frequency
Toolbar
Data Editor
Legend Box
Gallery
Color
Edit title
Point Labels
Font ...
Properties...
Statistical Studies
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
Arsenic 0 0 0 3 3 0 6 0 0 1 1 0 8 0 0 0 0 1 0 1
NROS_Arsenic 1 1 1 4 5 1 3 1 1 2 1 1 0 0 0 0 0 1 0 1

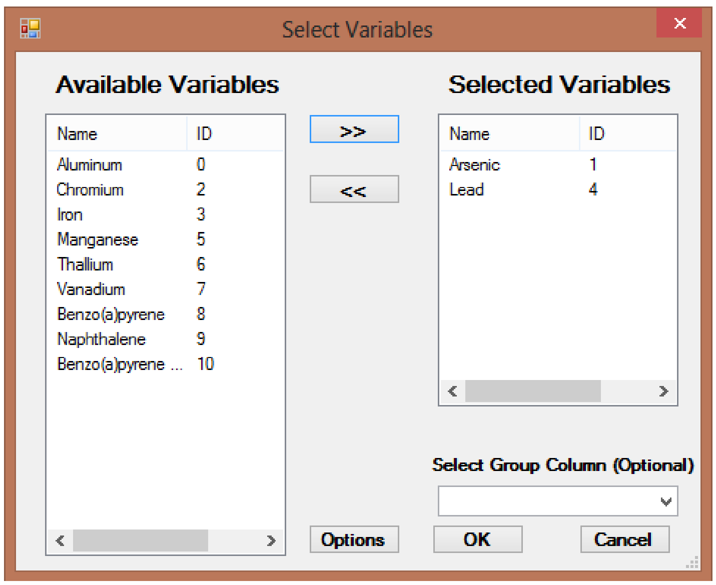

ProUCL 5.0 - [Box Plot Full_b.gst]
File Edit Stats/Sample Sizes BIS Simulator Graphs Statistical Tests Upper Limits/BTVs UCLs/EPCs Windows Help
Navigation Panel
Box Plot for Na
Action Level 20
Na
Toolbar
Data Grid
Legend Box
Gallery
Color
Edit title
Point Labels
Font ...
Properties...
Statistical Studies
Log Panel

Chapter 3

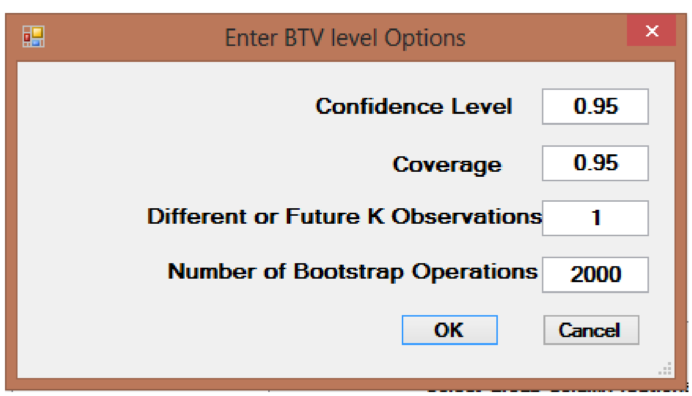
Select Variables Screen

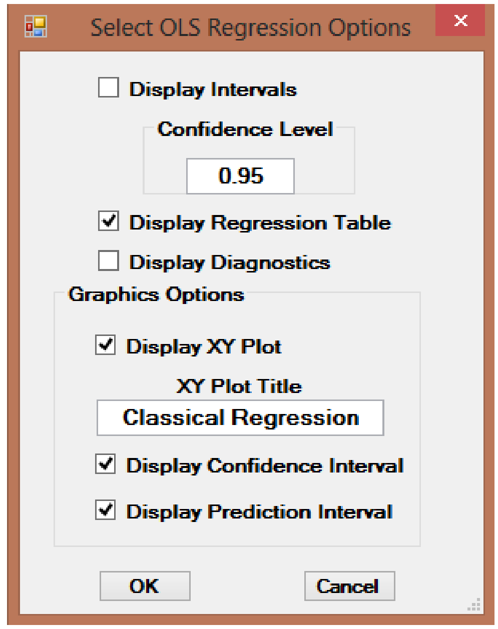
3.1 Select Variables Screen

- The **Select Variable** screen is associated with all modules of ProUCL.
- Variables need to be selected to perform statistical analyses.
- When the user clicks on a drop-down menu for a statistical procedure (e.g., UCLs/EPCs), the following window will appear.



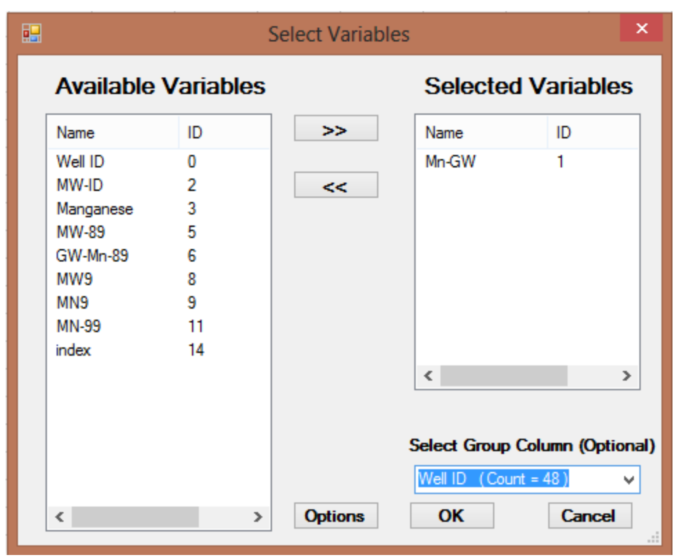
- The **Options** button is available in certain menus. The use of this option leads to another pop-up window such as shown below. This window provides the options associated with the selected statistical method (e.g., BTVs, OLS Regression).





- ProUCL can process multiple variables simultaneously. ProUCL software can generate graphs, and compute UCLs, and background statistics simultaneously for all selected variables shown in the right panel of the screen shot displayed on the previous page.

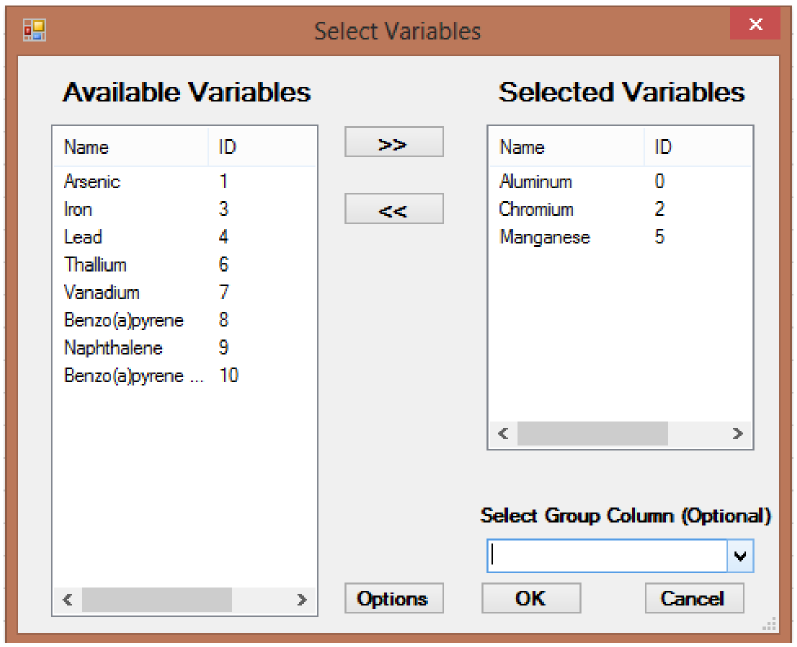
- If the user wants to perform statistical analysis on a variable (e.g., manganese) by a Group variable, click the arrow below the **Select Group Column (Optional)** to get a drop-down list of available variables from which to select an appropriate group variable. For example, a group variable (e.g., Well ID) can have alphanumeric values such as MW8, MW9, and MW1. Thus in this example, the group variable name, Well ID, takes 3 values: MW1, MW8, and MW9. The selected statistical method (e.g., GOF test) performs computations on data sets for all the groups associated with the selected group variable (e.g., Well ID)



- The Group variable is useful when data from two or more samples need to be compared.

- Any variable can be a group variable. However, for meaningful results, only a variable, that really represents a group variable (categories) should be selected as a group variable.

- The number of observations in the group variable and the number observations in the selected variables (to be used in a statistical procedure) should be the same. In the example below, the variable "Mercury" is not selected because the number of observations for Mercury is 30; in other words mercury values have not been grouped. The group variable and each of the selected variables have 20 data values.



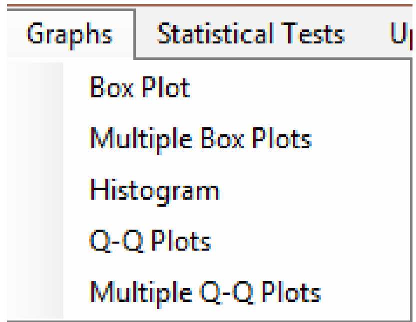
- As mentioned earlier, one should not assign any missing value such as a "Blank" for the group variable. If there is a missing value (represented by blanks, strings or 1E31) for a group variable, ProUCL will treat those missing values as a new group. As such, data values corresponding to the missing Group will be assigned to a new group.

- The **Group Option** is a useful tool for performing statistical tests and methods (including graphical displays) separately for each of the group (samples from different populations) that may be present in a data set. For example, the same data set may consist of samples from multiple populations. The graphical displays (e.g., box plots, Q-Q plots) and statistics of interest can be computed separately for each group by using this option.

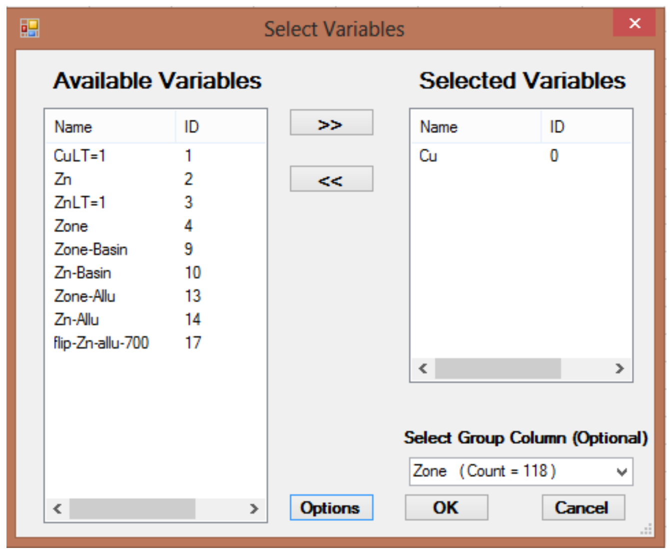
Notes: Once again, care should be taken to avoid misrepresentation and improper use of group variables. Do not assign any form of a missing value for the group variable.

3.1.1 Graphs by Groups

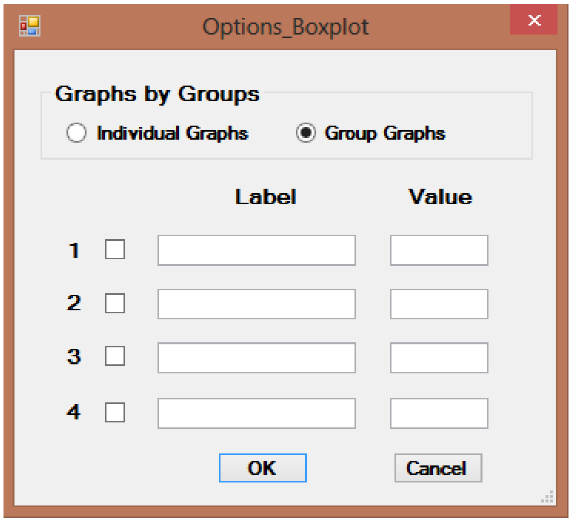
The following options are available to generate graphs by groups.



- Individual or multiple graphs (Q-Q plots, box plots, and histograms) can be displayed on a graph by selecting the **Group Column (Optional)** option shown as follows.



- An individual graph for each group (specified by the selected group variable) is produced by selecting the **Individual Graph** option; and multiple graphs (e.g., side-by-side box plots, multiple Q-Q plots on the same graph) are produced by selecting the **Group Graph** option as shown below. Using the **Group Graph** option, multiple graphs are displayed for all sub-groups included in the Group variable. This option is used when data are given in the same column and are classified by a group variable.



- Multiple graphs for selected variables are produced by selecting options: **Multiple Box Plots** or **Multiple Q-Q Plots**. Using the **Group Graph** option, multiple graphs for all selected variables are shown on the same graphical display. This option is useful when data (e.g., site lead and background lead) to be compared are given in different columns.

Notes: It should be noted that it is the users' responsibility to provide an adequate amount of detected data to perform the group operations. For example, if the user desires to produce a graphical Q-Q plot (using only detected data) with regression lines displayed, then there should be at least two detected points (to compute slope, intercept, and *sd*) in the data set. Similarly, if graphs are desired for each group specified by a Group ID variable, there should be at least two detected observations in each group specified by the Group ID variable. ProUCL displays a warning message (in orange) in the lower Log Panel of the ProUCL screen when not enough data are available to perform a statistical or graphical operation.

Chapter 4

General Statistics

The **General Statistics** option is available under the **Stats/Sample Sizes** module of ProUCL 5.0. This option is used to compute general statistics including simple summary statistics (e.g., mean, standard deviation) for all selected variables. In addition to simple summary statistics, several other statistics are computed for full uncensored data sets (**Full w/o NDs**), and for data sets with nondetect (**with NDs**) observations (e.g., estimates based upon the KM method). Two Menu options: **Full w/o NDs** and **With NDs** are available.

- **Full (w/o NDs)**: This option computes general statistics for all selected variables.

- **With NDs**: This option computes general statistics including the KM method based mean and standard deviations for all selected variables with ND observations.

Each menu option (**Full (w/o NDs)** and **With NDs**) has two sub-menu options:

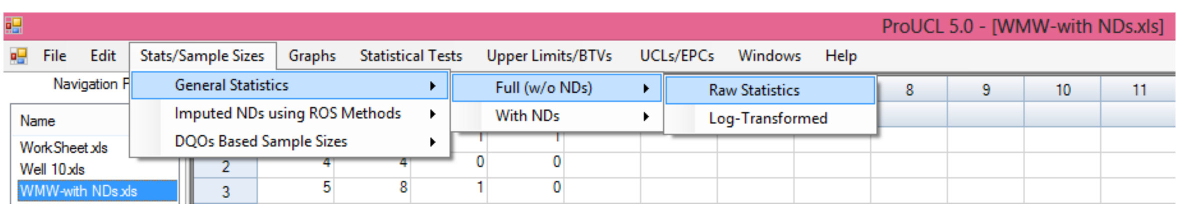
- Raw Statistics

- Log-Transformed

When computing general statistics for raw data, a message will be displayed for each variable that contains non-numeric values. The **General Statistics** option computes log-transformed (natural log) statistics only if all of the data values for the selected variable(s) are positive real numbers. A message will be displayed if non-numeric characters, zero, or negative values are found in the column corresponding to a selected variable.

4.1 General Statistics for Full Data Sets without NDs

1. Click **General Statistics ► Full (w/o NDs)**

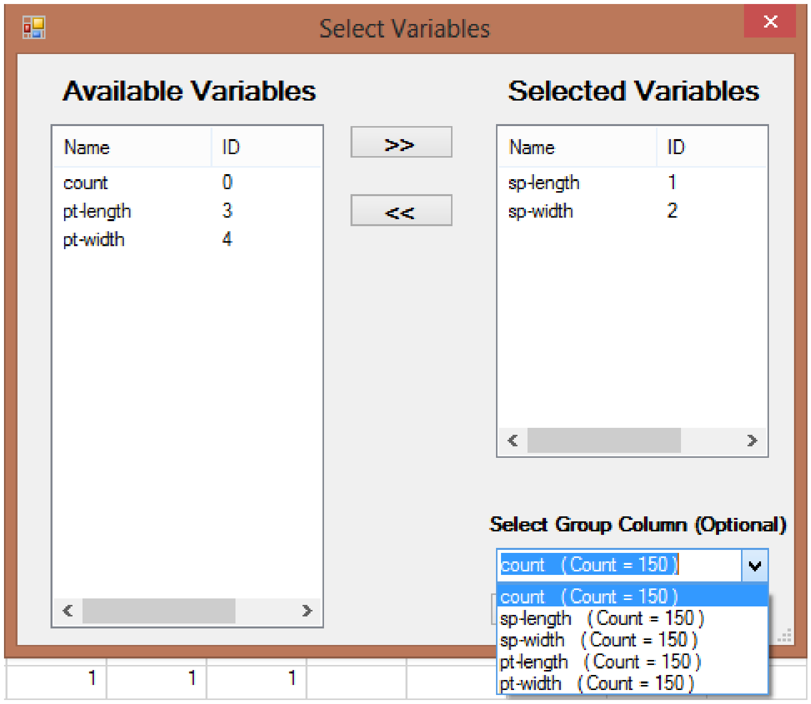


2. Select either **Log-Transformed** or **Raw Statistics** option.

3. The **Select Variables** screen (see Chapter 3) will appear.

- Select one or more variables from the **Select Variables** screen.

- If statistics are to be computed by a Group variable, then select a group variable by clicking the arrow below the **Select Group Column (Optional)** button. This will result in drop-down list of available variables, and select a proper group variable.



- Click on the **OK** button to continue or on the **Cancel** button to cancel the **General Statistics** option.

Raw Statistics

User Selected Options												
From File	FULLIRIS-nds.xls											
Full Precision	OFF											
From File: FULLIRIS-nds.xls												
Summary Statistics for Uncensored Data Sets												
Variable	**NumObs**	**# Missing**	**Minimum**	**Maximum**	**Mean**	**SD**	**SEM**	**MAD/0.675**	**Skewness**	**Kurtosis**	**CV**	
sp-length (1)	50	0	4.3	5.8	5.006	0.352	0.0498	0.297	0.12	-0.253	0.0704	
sp-length (2)	50	0	4.9	7	5.936	0.516	0.073	0.519	0.105	-0.533	0.087	
sp-length (3)	50	0	4.9	7.9	6.588	0.636	0.0899	0.593	0.118	0.0329	0.0965	
Percentiles for Uncensored Data Sets												
Variable	**NumObs**	**# Missing**	**10%ile**	**20%ile**	**25%ile(Q1)**	**50%ile(Q2)**	**75%ile(Q3)**	**80%ile**	**90%ile**	**95%ile**	**99%ile**	
sp-length (1)	50	0	4.59	4.7	4.8	5	5.2	5.32	5.41	5.61	5.751	
sp-length (2)	50	0	5.38	5.5	5.6	5.9	6.3	6.4	6.7	6.755	6.951	
sp-length (3)	50	0	5.8	6.1	6.225	6.5	6.9	7.2	7.61	7.7	7.802	

Log-Transformed Statistics

User Selected Options	
From File	FULLIRIS-nds.xls
Full Precision	OFF

From File: FULLIRIS-nds.xls

Summary Statistics for Uncensored Log-Transformed Data Sets

Variable	NumObs	# Missing	Minimum	Maximum	Mean	Variance	SD	MAD/0.675	Skewness	Kurtosis	CV
sp-length (1)	50	0	1.459	1.758	1.608	0.00497	0.0705	0.0605	-0.0553	-0.291	0.0438
sp-length (2)	50	0	1.589	1.946	1.777	0.00761	0.0872	0.0873	-0.0852	-0.463	0.0491
sp-length (3)	50	0	1.589	2.067	1.881	0.00943	0.0971	0.0885	-0.196	0.492	0.0516

Percentiles for Uncensored Log-Transformed Data Sets

Variable	NumObs	# Missing	10%ile	20%ile	25%ile(Q1)	50%ile(Q2)	75%ile(Q3)	80%ile	90%ile	95%ile	99%ile
sp-length (1)	50	0	1.524	1.548	1.569	1.609	1.649	1.671	1.688	1.724	1.749
sp-length (2)	50	0	1.683	1.705	1.723	1.775	1.841	1.856	1.902	1.91	1.939
sp-length (3)	50	0	1.758	1.808	1.829	1.872	1.932	1.974	2.029	2.041	2.054

4. The **General Statistics** screen (and all other output screens generated by other modules) shown above can be saved as an Excel 2003 (.xls) or 2007 (.xlsx) file. Click **Save** from the file menu.

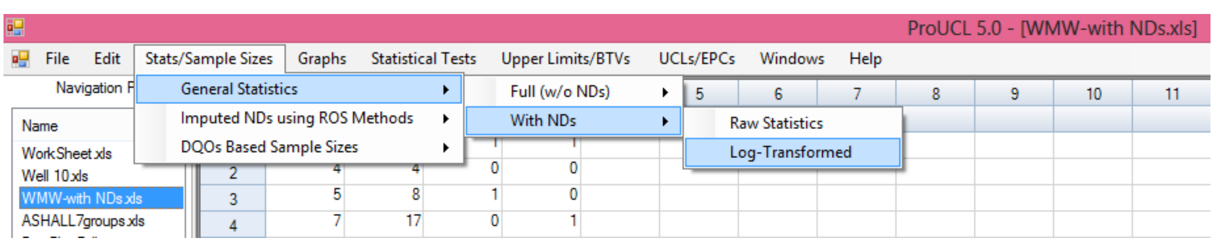
5. On the output screen shown above, most of the statistics are self explanatory and described in the ProUCL Technical Guide (EPA 2013, 2015). A couple of simple robust statistics (Hoaglin, Mosteller, and Tukey 1983) included in the above output are described as follows.

   MAD = Median absolute deviation

   MAD/0.675 = Robust and resistant (to outliers) estimate of variability, population standard deviation, σ

4.2 General Statistics with NDs

1. As above, Click **General Statistics ► With NDs**



2. Select either **Log-Transformed** or **Raw Statistics** option.

3. The **Select Variables** screen (Chapter 3) will appear.

- Select variable(s) from the list of variables.

- Only those variables that have ND values will be shown. The user should make sure that the variables with NDs are defined properly including the column showing the detection status of the various observations.

- If statistics are to be computed by a Group variable, then select a group variable by clicking the arrow below the **Select Group Column (Optional)** button. This will result in a drop-down list of available variables. Select a proper group variable.

- Click on the **OK** button to continue or on the **Cancel** button to cancel the summary statistics operations.

Raw Statistics – Data Set with NDs

User Selected Options	
From File	Zn-alluvial-fan-data.xls
Full Precision	OFF

From File: Zn-alluvial-fan-data.xls

Summary Statistics for Censored Data Set (with NDs) using Kaplan Meier Method

Variable	NumObs	# Missing	Num Ds	NumNDs	% NDs	Min ND	Max ND	KM Mean	KM Var	KM SD	KM CV
Cu (alluvial fan)	65	3	48	17	26.15%	1	20	3.608	13.08	3.616	1.002
Cu (basin trough)	49	1	35	14	28.57%	1	15	4.362	21.64	4.651	1.066

Summary Statistics for Raw Data Sets using Detected Data Only

Variable	NumObs	# Missing	Minimum	Maximum	Mean	Median	Var	SD	MAD/0.675	Skewness	CV
Cu (alluvial fan)	48	3	1	20	4.146	2	16.04	4.005	1.483	2.256	0.966
Cu (basin trough)	35	1	1	23	5.229	3	27.18	5.214	2.965	1.878	0.997

Percentiles using all Detects (Ds) and Non-Detects (NDs)

Variable	NumObs	# Missing	10%ile	20%ile	25%ile(Q1)	50%ile(Q2)	75%ile(Q3)	80%ile	90%ile	95%ile	99%ile
Cu (alluvial fan)	65	3	1	2	2	3	5	7	10	15.2	20
Cu (basin trough)	49	1	1	2	2	4	8	9.4	12.4	15	20.12

- The **Summary Statistics** screen shown above can be saved as an Excel 2003 or 2007 file. Click **Save** from the file menu.

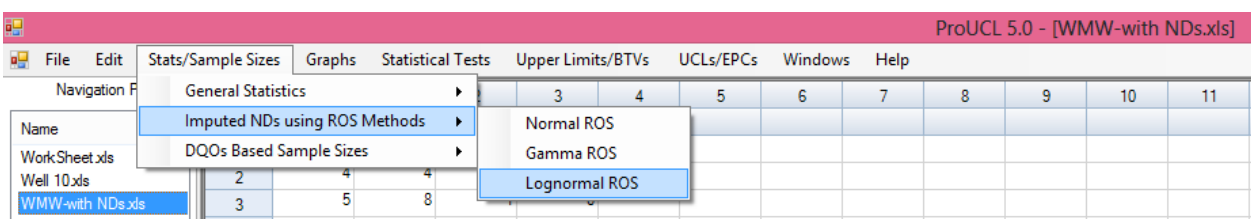
Chapter 5

Imputing Nondetects Using ROS Methods

The imputing of NDs using regression on order statistics (ROS) methods option is available under the **Stats/Sample Sizes** module of ProUCL 5.1. This option is provided for advanced users who want to use the detected and imputed NDs data for exploratory and data mining purposes on multivariate data sets. For exploratory methods, such as principal component analysis (PCA), cluster, and discriminant analysis to gain additional insight into potential structures and patterns present in a multivariate (more than one variable) data set, one may want to use imputed values in graphical displays (line graphs, scatter plots, boxplots etc.) and in the analyses. To derive conclusions based upon multivariate data sets with nondetects, the developers suggest the use of the KM method based covariance or correlation matrix to perform PCA and regression analysis. These methods are beyond the scope of the ProUCL software which deals only with univariate methods. The details of computing an Orthogonalized Kettenring and Gnanadesikan (OKG) positive definite KM matrix can be found in Maronna, Martin, and Yohai (2006) and in Scout 2008 Version 1.0 guidance documents (2009) which can be downloaded from the EPA Site (http://archive.epa.gov/esd/archive-scout/web/html/). One may not use ROS imputed data to perform parametric statistical tests such as t-test and ANOVA test without further investigation. These issues require further research to evaluate decision errors associated with conclusions derived using such methods.

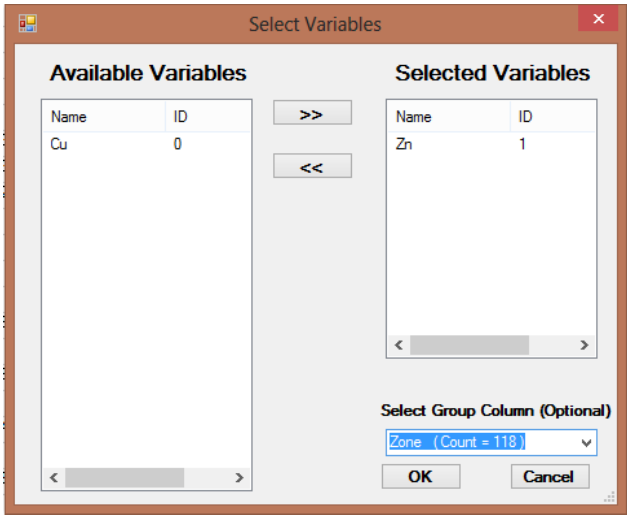
The ROS methods can be used to impute ND observations using a normal, lognormal, or gamma model. ProUCL has three ROS estimation methods that can be used to impute ND observations. The use of this option generates additional columns consisting of all imputed NDs and detected observations. These columns are appended to the existing open spreadsheet file. The user should save the updated file if they want to use the imputed data for their other application(s) such as PCA or discriminant analysis. It is not easy to perform multivariate statistical methods on data sets with NDs. The availability of imputed NDs in a data file helps the advanced users who want to use exploratory methods on data sets with ND observations. Like other statistical methods in ProUCL, NDs can also be imputed by a group variable. One can impute NDs using the following steps.

1. Click **Imputed NDs using ROS Methods ► Lognormal ROS**



2. The **Select Variables** screen (Chapter 3) will appear.

- Select one or more variable(s) from the **Select Variables** screen; NDs can be imputed using a group variable as shown in the following screen shot.



- Click on the **OK** button to continue or on the **Cancel** button to cancel the option.

Output Screen for ROS Est. NDs (Lognormal ROS) Option

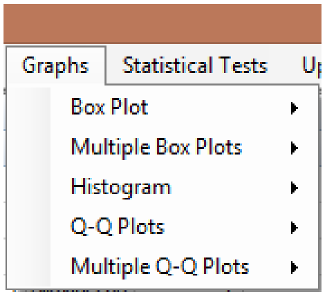
0	1	2	3	4	5	6
Cu	Zn	Zone	D_Cu	D_Zn	LnROS_Zn (alluvial fan)	LnROS_Zn (basin trough)
1	10	Alluvial Fan	0	0	2.12437794466611	20
1	9	Alluvial Fan	0	1	9	10
3		Alluvial Fan	1		1.000000E+031	60
3	5	Alluvial Fan	1	1	5	20
5	18	Alluvial Fan	1	1	18	12
1	10	Alluvial Fan	1	0	2.7045642735474	8
4	12	Alluvial Fan	1	1	12	3.48713118440742
4	10	Alluvial Fan	1	1	10	14
2	11	Alluvial Fan	1	1	11	4.98477186220711
2	11	Alluvial Fan	1	1	11	17
1	19	Alluvial Fan	1	1	19	1.87132713438924
2	8	Alluvial Fan	1	1	8	11
5	3	Alluvial Fan	0	0	2.49463676896719	5
11	10	Alluvial Fan	1	0	3.1603475071042	12
1	10	Alluvial Fan	0	0	3.55892730586941	4
2	10	Alluvial Fan	1	1	10	3
2	10	Alluvial Fan	1	1	10	6
2	10	Alluvial Fan	1	1	10	3
2	10	Alluvial Fan	1	1	10	15
20	10	Alluvial Fan	0	0	3.92469067412296	13
2	10	Alluvial Fan	1	1	10	4
2	10	Alluvial Fan	1	0	4.26969100939485	20
3	10	Alluvial Fan	1	1	10	20
3	10	Alluvial Fan	1	0	4.60094330444612	70
	10	Alluvial Fan		1	10	60
20	10	Alluvial Fan	0	0	4.92298559179133	40
10	10	Alluvial Fan	0	1	10	30
7	10	Alluvial Fan	1	1	10	40
5	20	Alluvial Fan	1	1	20	17

Notes: For grouped data, ProUCL generates a separate column for each group in the data set as shown in the above table. Columns with a similar naming convention are generated for each selected variable and distribution using the ROS option.

Chapter 6

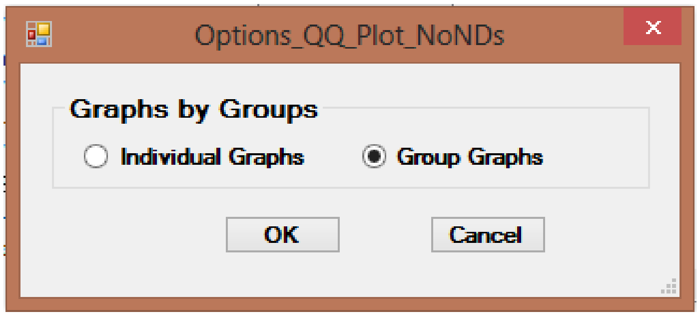
Graphical Methods (Graph)

The graphical methods described here are used as exploratory tools to get some idea about data distributions (e.g., skewed, symmetric), potential outliers and/or multiple populations present in a data set. The following graphical methods are available under the **Graphs** option of ProUCL 5.1

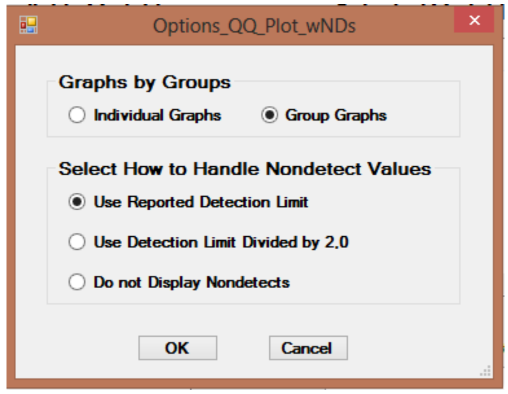


- All graphical displays listed above can be generated using uncensored full data sets (**Full w/o NDs**) as well as left-censored data sets with nondetect (**With NDs**) observations. On box plot graphs for data sets with NDs, a horizontal line is also displayed at the highest RL/DL associated with ND observations.

- Q-Q Plots and Histograms: Q-Q plots and histograms can be generated individually as well as by using a Group variable. Graphs generated using the **Group Graphs** option shown below is useful when data for selected variable(s) are given in the same column (stacked data) categorized by a Group ID.



- For data sets with NDs, three options described below are available to draw Q-Q plots and histograms. Specifically, these graphs are displayed only for detected values, or with NDs replaced by 1/2DL values, or with NDs replaced by the respective DLs. The statistics displayed on a Q-Q plot (mean, *sd*, slope, intercept) are computed according to the selected method. On Q-Q plots, ND values are displayed using a different symbol. The exploratory Q-Q plots described here do not require any placeholders for NDs. These graphs are used only to determine the distribution of detected values and to identify potential outliers and/or multiple populations present in a data set. On histograms, the user can change the number of bins (more bins, less bins) used to generate histograms.



Do not Display Nondetects: Selection of this option excludes all NDs from a graphical method (Q-Q plots and histograms) and plots only detected values. The statistics shown on Q-Q plots are computed only using the detected data.

Use Reported Detection Limit: Selection of this option treats DLs/RLs as detected values associated with the ND values. The graphs are generated using the numerical values of detection limits and statistics displayed on Q-Q plots are computed accordingly.

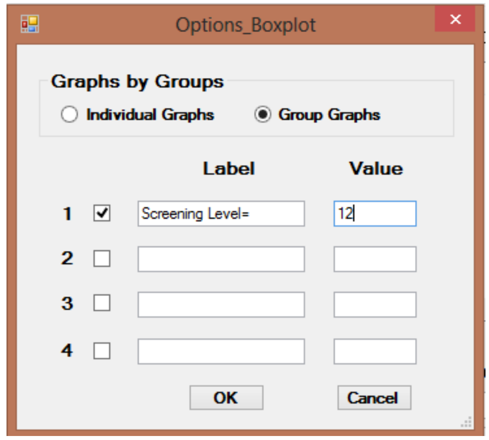
Use Detection Limit Divided by 2.0: Selection of this option replaces the DLs with their half values. All Q-Q plots and histograms are generated using the half detection limits and detected values. The statistics displayed on Q-Q plots are computed accordingly.

- For data sets in different columns, one can use the **Multiple Q-Q Plots** option. By default, this option will display multiple Q-Q plots for all selected variables on the same graph. One can also generate multiple Q-Q plots by using a group variable.

- Box Plot: Like Q-Q plots, box plots can also be generated by a Group variable. This option is useful when all data are listed in the same column (stacked data) categorized by a Group ID variable. On box plots with NDs, a horizontal line is displayed at the highest detection limit level. ProUCL 5.1 constructs a box plot using all detected and nondetected (using associated DL values) values. A horizontal line is displayed at the highest detection limit. Box Plots are generated using ChartFx, a software used in the development of ProUCL 5.1.

- Multiple Box Plots: For data in different columns, one can use the **Multiple Box Plots** option to display multiple box plots for all selected variables on the same graph. One can also generate multiple box plots by using a group variable.

- Box Plots have an optional feature, which can be used to draw up to four (4) horizontal lines at pre-established screening levels or at statistical limits (e.g., upper limits) computed using a background data set. This option can be used when box plots are generated using onsite data and one may be interested in comparing onsite data with background threshold values and/or pre-established screening levels. This type of box plot represents a visual comparison of site data with background threshold values and/or other action levels. Up to four (4) values can be displayed on a box plot as shown below. If the user inputs a value in the value column, the check box in that row will get activated. For example, the user may want to display horizontal lines at a background UTL95-95 or some pre-established action level(s) on box plots generated using AOCs data.



6.1 Box Plot

A brief description of the method used to generate Tukey's box plot (also known as box and whisker plot) is described first.

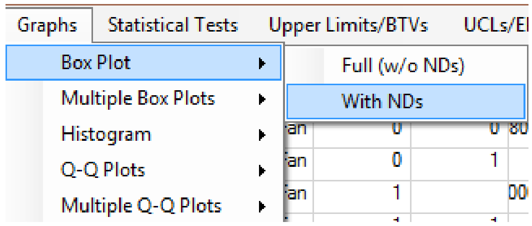
Box Plot (Box and Whiskers Plot): A box plot (box and whiskers plot) represents a convenient exploratory tool and provides a quick five-point summary of a data set. In statistical literature, one can find several ways to generate box plots. The practitioners may have their own preferences to use one method over the other. Box plots are well documented in the statistical literature and a description of box plots can be easily obtained by surfing the net. Therefore, a detailed description about the generation of box plots is not provided in ProUCL guidance documents.

All box plot methods including the one in ProUCL represent five-point summary graphs including: the lowest and the highest data values, median (50^{th} percentile=second quartile, Q2), 25^{th} percentile (lower quartile, Q1), and 75^{th} percentile (upper quartile, Q3). A box and whisker plot also provides information about the degree of dispersion (interquartile range (IQR) = Q3-Q1=length/height of the box in a box plot), the degree of skewness (suggested by the length of the whiskers) and unusual data values known as outliers. Specifically, ProUCL (and various other software packages) use the following to generate a box and whisker plot.

- Q1= 25^{th} percentile, Q2= 50^{th} (median), and Q3 = 75^{th} percentile
- Interquartile range= IQR = Q3-Q1 (the height of the box in a box plot)
- Lower whisker starts at Q1 and the upper whisker starts at Q3.
- Lower whisker extends up to the lowest observation or (Q1 - 1.5 * IQR) whichever is higher
- Upper whisker extends up to the highest observation or (Q3 + 1.5 * IQR) whichever is lower
- Horizontal bars (also known as fences) are drawn at the end of whiskers
- Observations lying outside the fences (above the upper bar and below the lower bar) represent potential outliers

ProUCL uses a couple of development tools such as FarPoint spread (for Excel type input and output operations) and ChartFx (for graphical displays). ProUCL generates box plots using the built-in box plot feature in ChartFx. The programmer has no control over computing the statistics (e.g., Q1, Q2, Q3, IQR) using ChartFx. Boxplots generated by ProUCL can slightly differ from box plots generated by other programs (e.g., Excel). However, for all practical and exploratory purposes, box plots in ProUCL are equally good (if not better) than those available in the various commercial software packages for exploring data distribution (skewed or symmetric), identifying outliers, and comparing multiple groups (main objectives of box plots in ProUCL). More details about Box Plots can be found in Section 1.16 of Chapter 1 of this document.

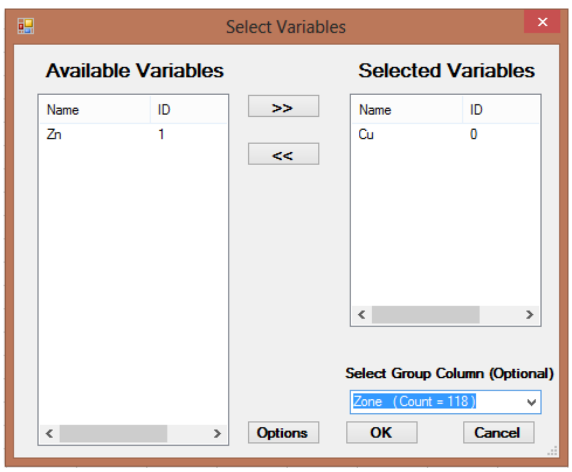
1. Click **Graphs ► Box Plot**



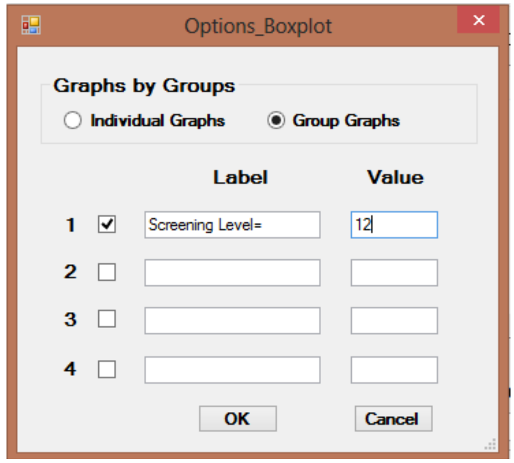
2. The **Select Variables** screen (Chapter 3) will appear.

- Select one or more variable(s) from the **Select Variables** screen.

- If graphs are to be produced by using a Group variable, select a group variable by clicking the arrow below the **Select Group Column (Optional)** button. This will result in a drop-down list of available variables. The user should select an appropriate variable representing a group variable as shown below.



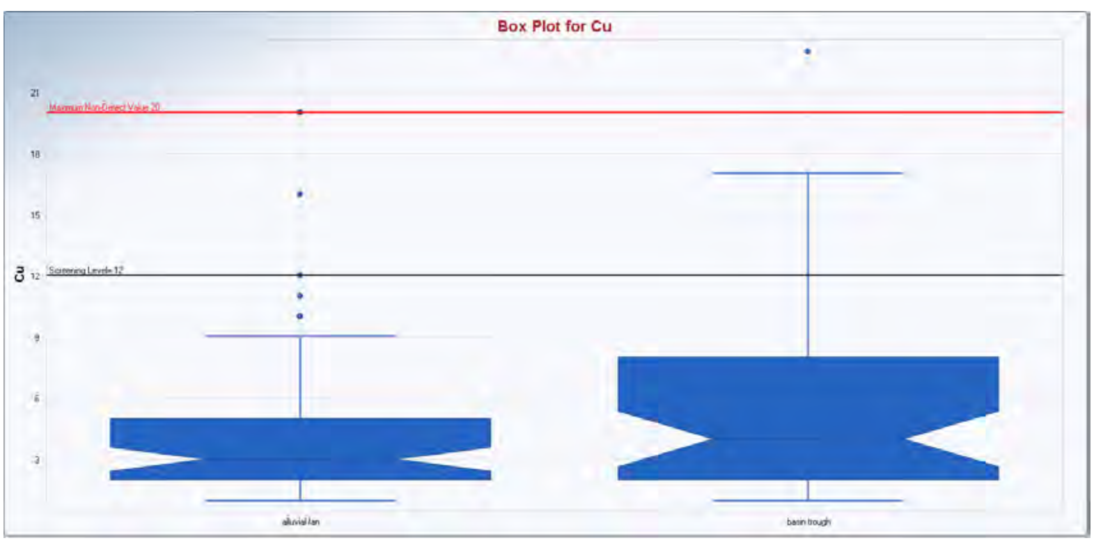
The default option for **Graph by Groups** is **Group Graphs**. This option produces side-by-side box plots for all groups included in the selected Group ID Column (e.g., Zone here). The **Group Graphs** option is used when multiple graphs categorized by a group variable need to be produced on the same graph. The **Individual Graphs** option generates individual graphs for each selected variable or one box plot for each group for the variable categorized by a Group ID column (variable).



- While generating box plots, one can display horizontal lines at specified screening levels or a BTV estimate (e.g., UTL95-95) computed using a background data set. For data sets with NDs, a horizontal line is also displayed at the largest reported DL associated with a ND value. The use of this option may provide information about the analytical methods used to analyze field samples.

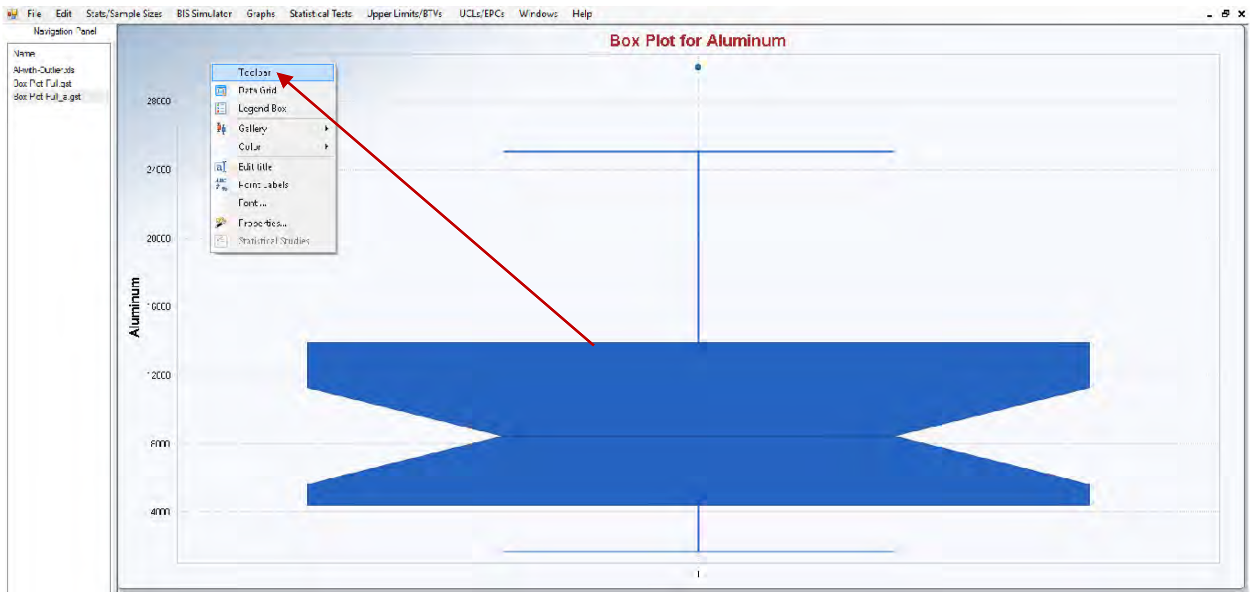
- Click on the **OK** button to continue or on the **Cancel** button to cancel the Box Plot (or other selected graphical) option.

Box Plot Output Screen (Group Graph)
Selected options: Label (Screening Level), Value (12)

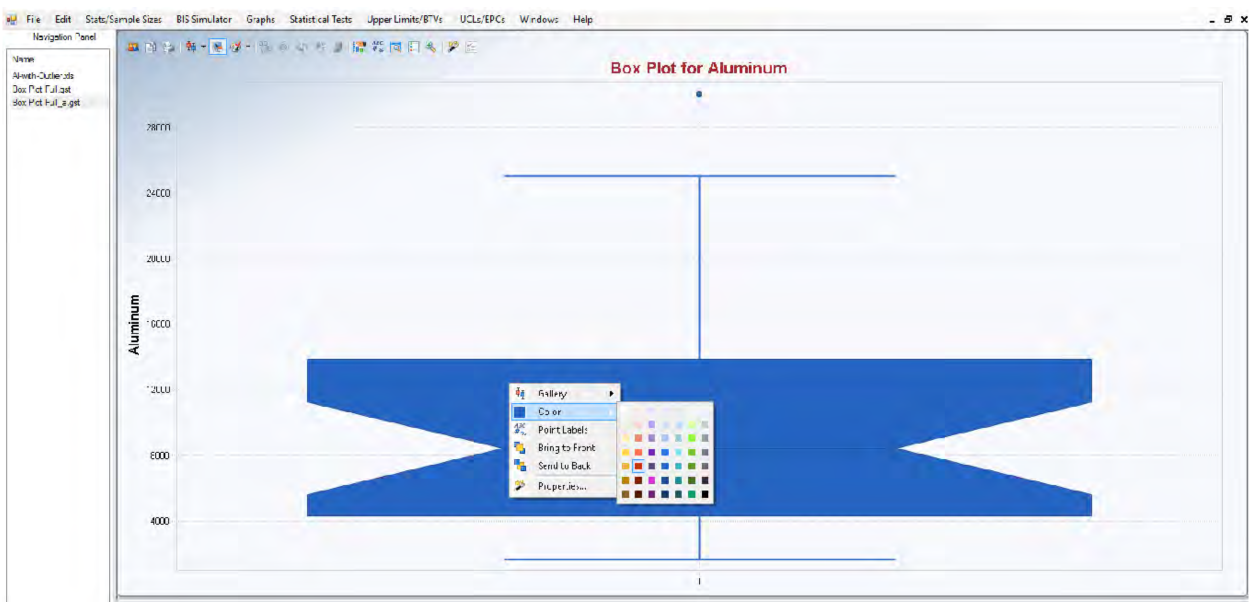


Making Changes in Graphs using Toolbar

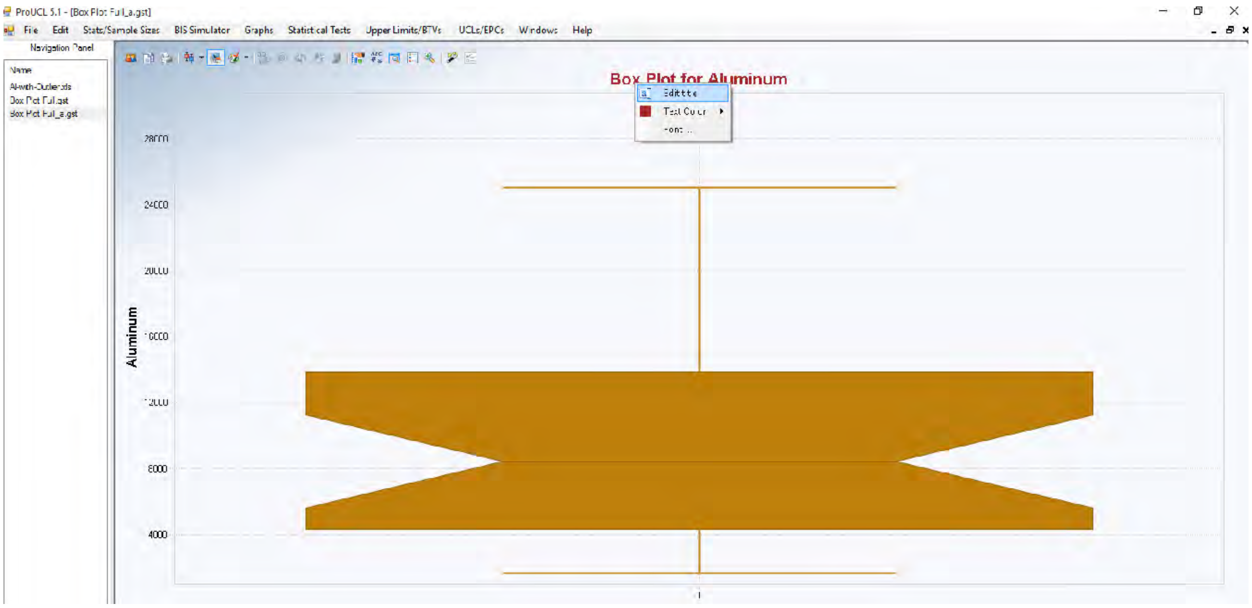
One can use the toolbar to make changes in a graph generated by ProUCL. The toolbar can be activated by right clicking the mouse on your graph. The context menu on the box plot shown below appears. By using the context menu, one can change color, title, font size, legend box and label points. For example, one can edit the title by clicking title in the context menu. These are typical windows operations which can also be used in ProUCL. However, it should be pointed out that options which affect the computation of statistics displayed on a graph are not wired and can yield incorrect results. For example, changing scales along the x-axis or y-axis (e.g., to log scale) will not automatically displayed statistics in the changed log- scale. The resulting graph using options that affect computed statistics will be incorrect and should be avoided. These operations are illustrated by several screen captures displayed as follows.



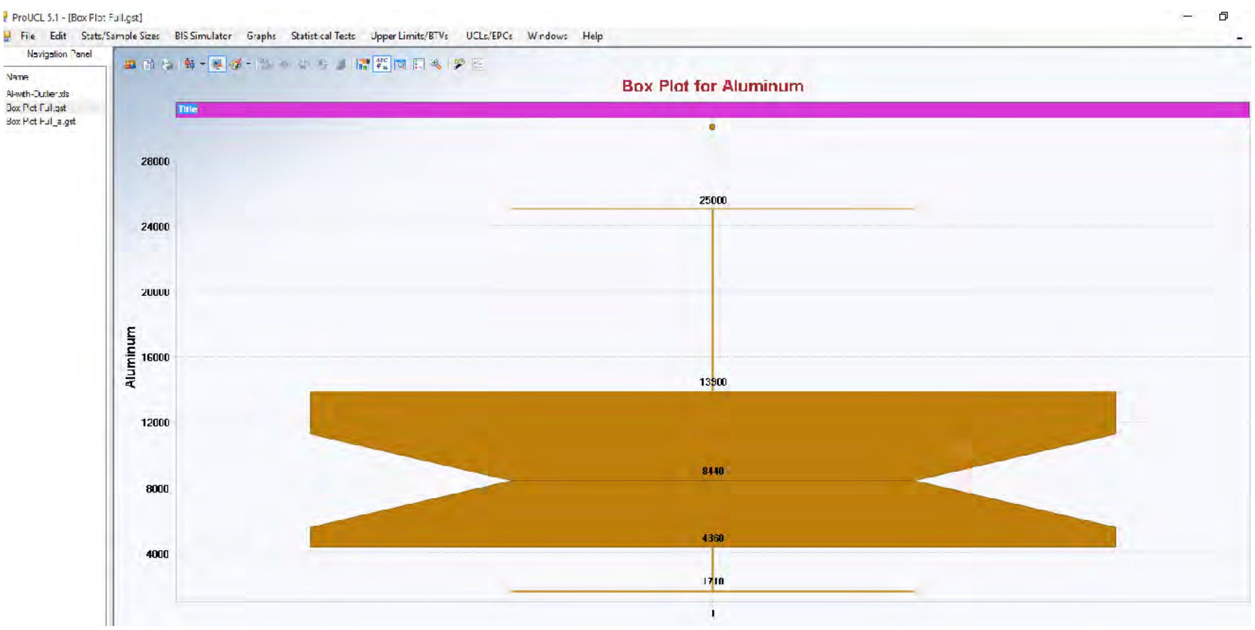
Activating the toolbar shown above.



Changing color of the graph shown in the above graph.



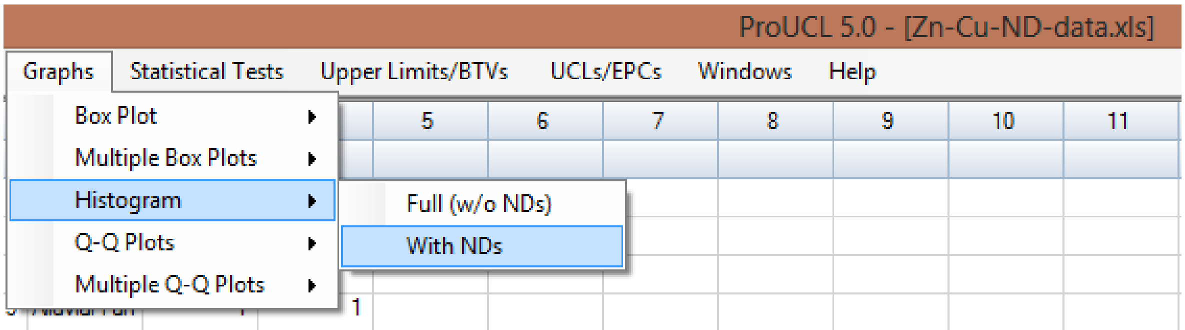
Changing title of the graph.



Edit the title of the graph.

6.2 Histogram

1. Click **Graphs ► Histogram**

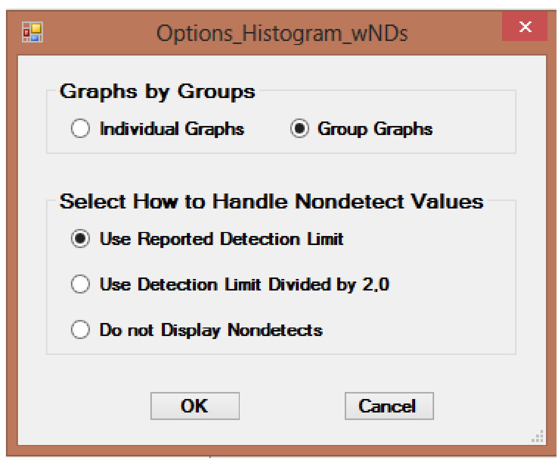


2. The **Select Variables** screen (Chapter 3) will appear.

- Select one or more variable(s) from the **Select Variables** screen.

- If graphs have to be produced by using a Group variable, then select a group variable by clicking the arrow below the **Select Group Column (Optional)** button. This will result in a drop-down list of available variables. The user should select an appropriate variable representing a group variable as shown below.

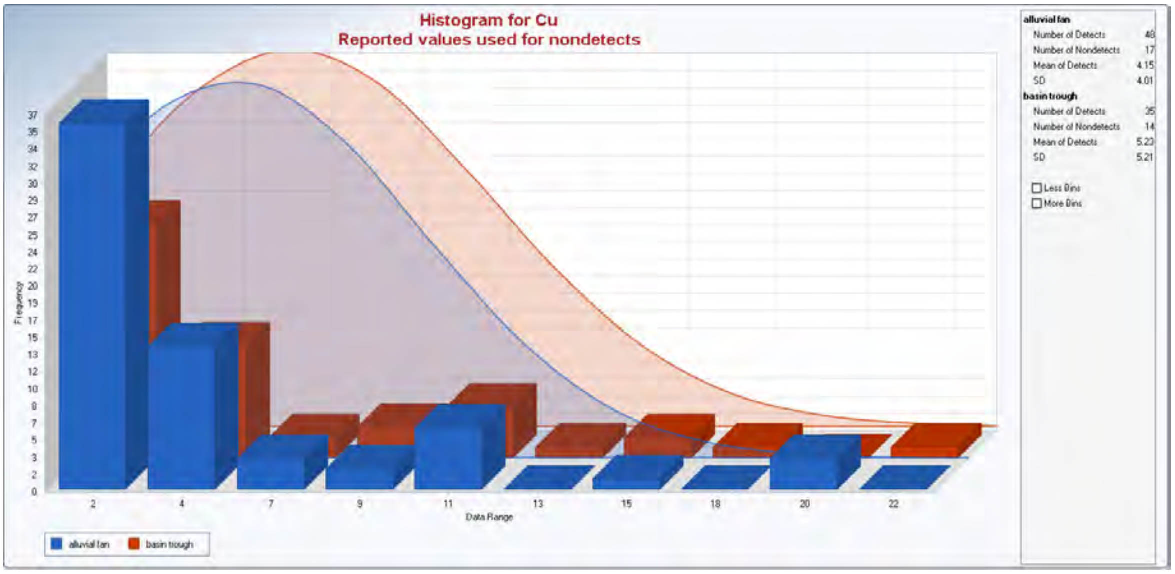
- When the option button is clicked for data sets with NDs, the following window will be shown. By default, histograms are generating using the RLs for NDs.



- The default selection for histograms (and for all other graphs) by a group variable is **Group Graphs**. This option produces multiple histograms on the same graph. If histograms are needed to be displayed individually, the user should check the radio button next to **Individual Graphs**.

- Click on the **OK** button to continue or on the **Cancel** button to cancel the histogram (or other selected graphical) option.

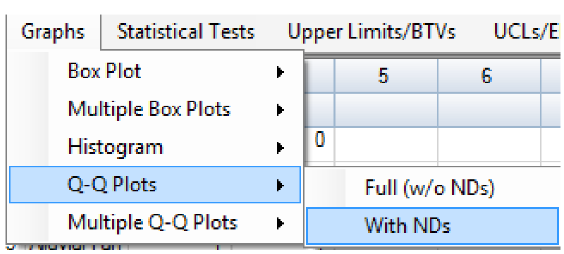
Histogram Output Screen
Selected options: Group Graphs



<u>Notes:</u> ProUCL does not perform any GOF tests when generating histograms. Histograms are generated using the development software ChartFx and not many options are available to alter the histograms. The labeling along the x-axis is done by the development software and it is less than perfect. However, if one hovers the mouse on a bar, relevant statistics (e.g., begin point, midpint and end point) about the bar will appear on the screen. The **Histogram** option automatically generates a normal probability density function (pdf) curve irrespective of the data distribution. At this time, ProUCL 5.1 does not display a pdf curve for any other distribution (e.g., gamma) on a historgram. The user can increase or decrease the number of bins to be used in a histogram.

6.3 Q-Q Plots

1. **Click** Graphs ► Q-Q Plots**. When that option button is clicked, the following window will be shown.**



2. Q-Q Plots can be generated for data sets **With NDs** and without NDs [**Full (w/o NDs)**].

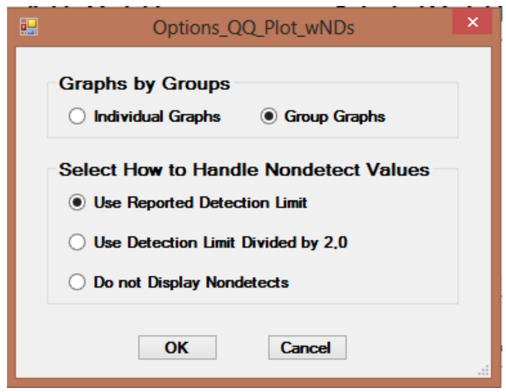
 - Select either **Full (w/o NDs)** or **With NDs** option.

 - The **Select Variables** screen (Chapter 3) will appear.

- Select one or more variable(s) from the **Select Variables** screen.

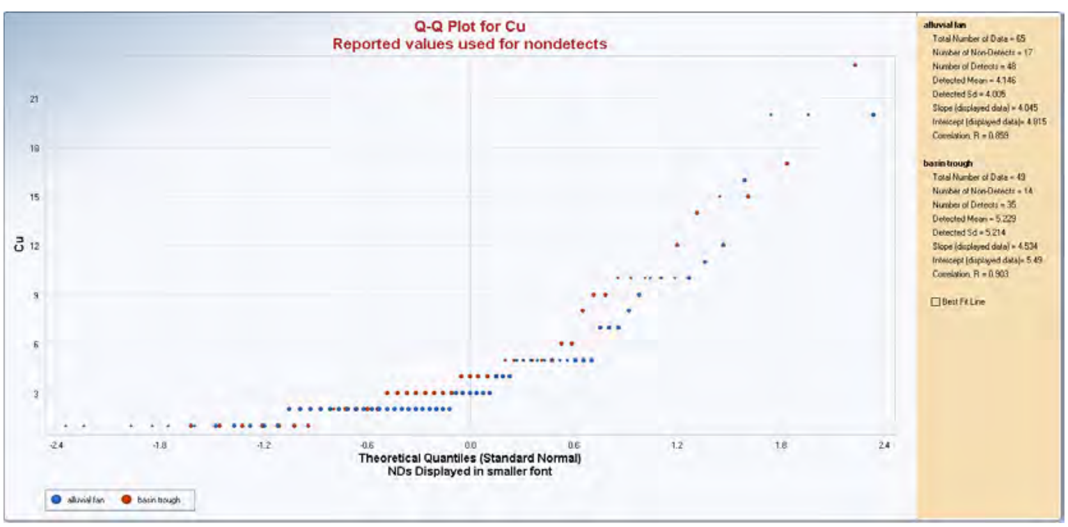
- If graphs have to be produced by using a group variable, then select a group variable by clicking the arrow below the **Select Group Column (Optional)** button. This will result in a drop-down list of available variables. The user should select and click on an appropriate variable representing a group variable as shown below.

- Click on the **OK** button to continue or on the **Cancel** button to cancel the selected Q-Q plots option. The following options screen appears providing choices on how to treat NDs. The default option is to use the reported values for all NDs.



- Click on the OK button to continue or on the Cancel button to cancel the selected Q-Q plots option. The following Q-Q plot appears when used on the copper concentrations of two zones: Alluvial Fan and Basin Trough.

Output Screen for Q-Q plots (With NDs)
Selected options: Group Graph, No Best Fit Line



Note: The font size of ND values is smaller than that of the detected values.

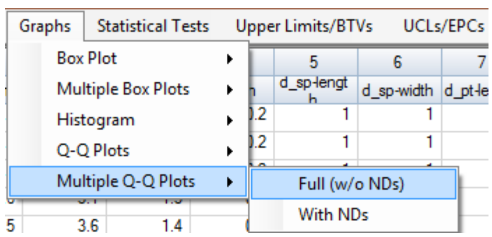
6.4 Multiple Q-Q Plots

6.4.1 Multiple Q-Q plots (Uncensored data sets)

1. ***Click** Graphs ► Multiple Q-Q Plots*

2. **Multiple Q-Q Plots can be generated for data sets** With NDs **and without NDs [**Full (w/o NDs)**].**

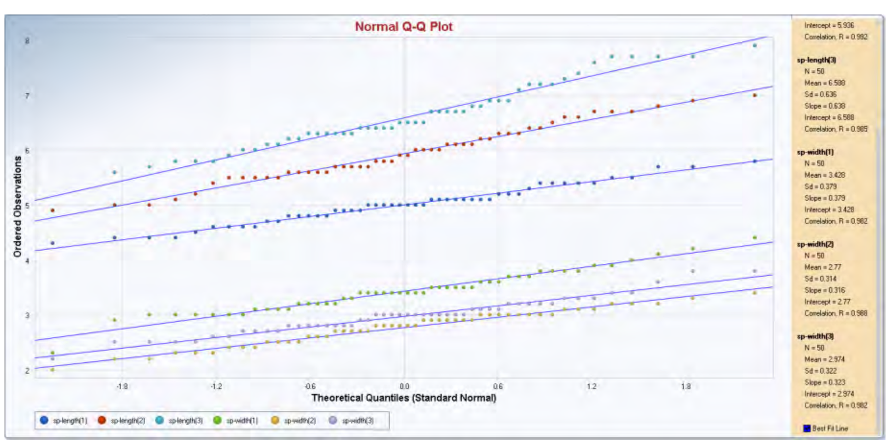
- When that **Option** button is clicked, the following window will be shown.



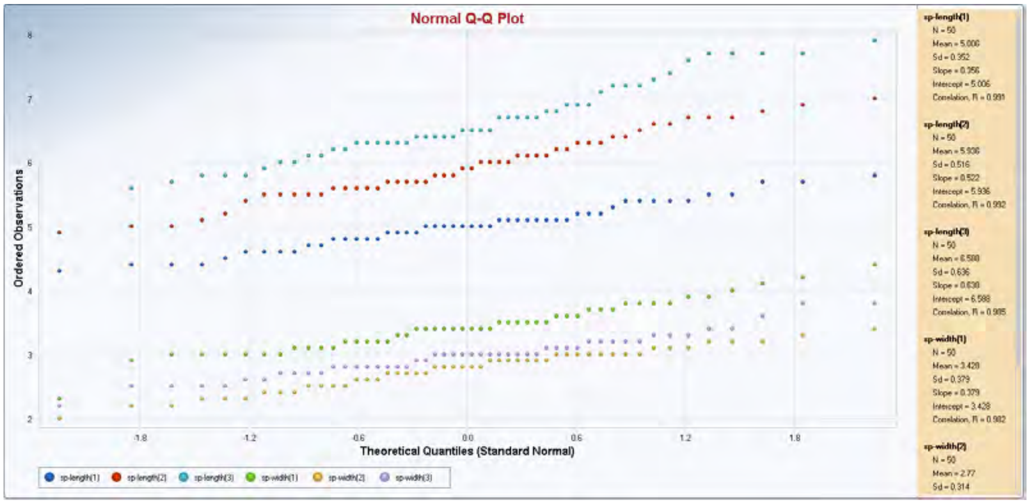
- Select either **Full (w/o NDs)** or **With NDs**.
- The **Select Variables Screen** (Chapter 3) will appear.
- Select one or more variable(s) from the **Select Variables** screen.
- If graphs have to be produced by using a Group variable, then select a group variable by clicking the arrow below the **Select Group Column (Optional)** button. This will result in a drop-down list of available variables. The user should select and click on an appropriate variable representing a group variable as shown below.
- Click **OK** to continue or **Cancel** button to cancel the selected Multiple Q-Q Plots option.

Example 6-1: The following graph is generated by using Fisher's (1936) data set for 3 Iris species.

Output Screen for Multiple Q-Q Plots (Full w/o NDs)
Selected Options: Group Graph, Best Fit Line



If the user does not want the regression lines shown above, click on the **Best Fit Line** and all regression lines will disappear as shown below.



Notes: For Q-Q plots and Multiple Q-Q plots option, for both "Full" as well as for data sets "With NDs," the values along the horizontal axis represent quantiles of a standardized normal distribution (Normal distribution with mean=0 and standard deviation=1). Quantiles for other distributions (e.g., Gamma distribution) are used when using the **Goodness-of-Fit (GOF, G.O.F.)** test option.

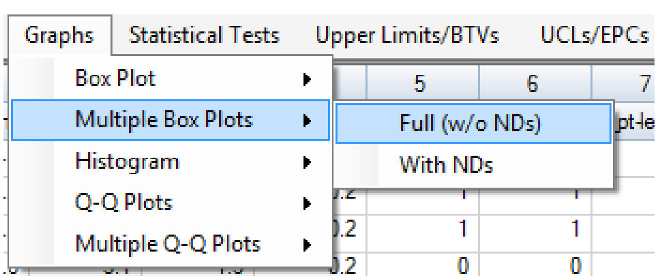
6.5 Multiple Box Plots

6.5.1 Multiple Box plots (Uncensored data sets)

1. ***Click** Graphs ► Multiple Box Plots*

2. **Multiple Q-Q Plots can be generated for data sets** With NDs **and without NDs [**Full (w/o NDs)**].**

- When the option button is clicked, the following window will be shown.



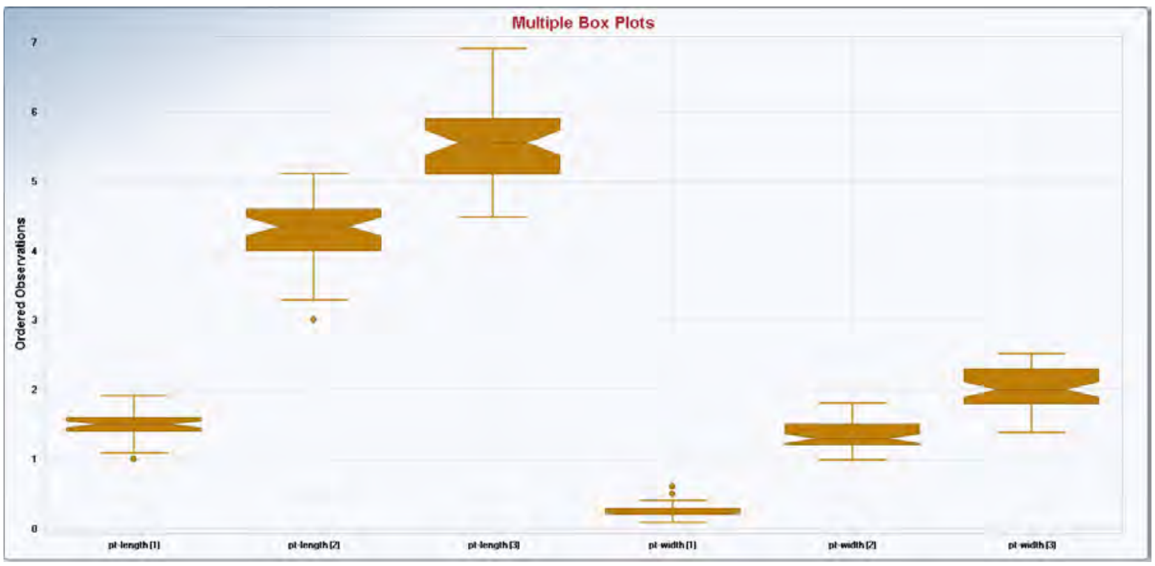
- Select either Full (w/o NDs) or With NDs.
- The **Select Variables** screen (Chapter 3) will appear.
- Select one or more variable(s) from the **Select Variables** screen.

- If graphs have to be produced by using a Group variable, then select a group variable by clicking the arrow below the **Select Group Column (Optional)** button. This will result in a drop-down list of available variables. The user should select and click on an appropriate variable representing a group variable as shown below.

- Click on the **OK** button to continue or on the **Cancel** button to cancel the selected Multiple Box Plots options. The following graph is generated by using the above options.

Example 6-1 (continued): The following graph is generated by using the above options on Fisher's (1936) Iris data set collected from 3 species of Iris flower.

Output Screen for Multiple Box Plots (Full w/o NDs)
Selected options: Group Graph



Chapter 7

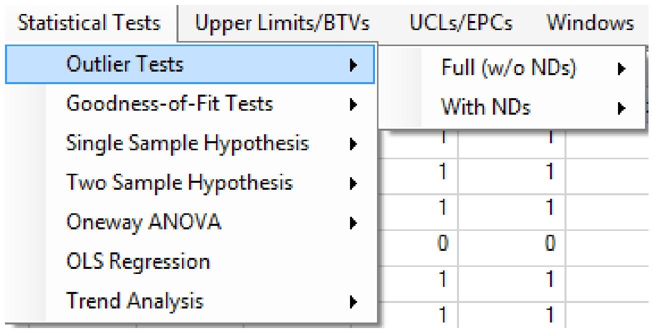
Classical Outlier Tests

Outliers are inevitable in data sets originating from environmental applications. In addition to informal graphical displays (e.g., Q-Q plots and box plots) and classical outlier tests (Dixon test, Rosner test), there exist several robust outlier identification methods (e.g., Biweight, Huber, PROP, MCD) for identifying any number of multiple outliers present in data sets of various sizes (Scout 2008; EPA 2009). It is well known that the classical outlier tests: Dixon test and Rosner test suffer from masking (e.g., extreme outliers may mask intermediate outliers) effects. The use of robust outlier identification procedures is recommended for identifying multiple outliers, especially when dealing with multivariate (having multiple constituents) data sets. However, those preferred and more efficient robust outlier identification methods are beyond the scope of ProUCL 5.1. Several robust outlier identification methods (e.g., based upon Biweight, Huber, and PROP influence functions, Singh and Nocerino 1995) are available in the Scout 2008 v1.0 software package (EPA, 2009).

The two classical outlier tests: Dixon and Rosner tests (EPA 2006a; Gilbert 1987) are available in ProUCL 4.0 and higher versions of the ProUCL software. These tests can be used on data sets with and without ND observations. These tests require the assumption of normality of the data set <u>without</u> the outliers; as data sets consisting of outliers seldom follow a normal distribution. It should be noted that in environmental applications, one of the objectives is to identify high outlying observations that might be present in the right tail of a data distribution, as those observations often represent contaminated locations requiring further investigations. Therefore, for data sets with NDs, two options are available in ProUCL to deal with data sets with outliers. These options are: 1) exclude NDs and 2) replace NDs by DL/2 values. These options are used only to identify outliers and not to compute any estimates and limits used in decision-making processes. To compute the various statistics of interest, ProUCL uses rigorous statistical methods suited for left-censored data sets with multiple DLs.

It is suggested that the outlier identification procedures be supplemented with graphical displays such as <u>normal</u> Q-Q plots and box plots. On a normal Q-Q plot, observations that are well-separated from the bulk of the data typically represent potential outliers needing further investigation. Also, significant and obvious jumps and breaks in a normal Q-Q plot can be indications of the presence of more than one population and/or data gaps due to lack of enough data points (data sets of smaller sizes). Data sets of large sizes (e.g., >100) exhibiting such behavior on Q-Q plots may need to be partitioned out into component sub-populations before estimating EPCs or BTVs.

Outlier tests in ProUCL 5.1 are available under the **Statistical Tests** module.

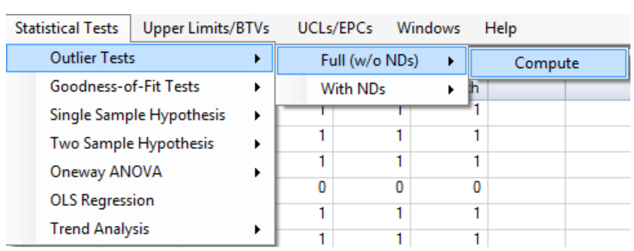


Dixon's Outlier Test (Extreme Value Test): Dixon's test is used to identify statistical outliers when the sample size is ≤ 25. This test identifies outliers or extreme values in the left tail (Case 2) and also in the right tail (Case 1) of a data distribution. In environmental data sets, outliers found in the right tail, potentially representing impacted locations, are of interest. The Dixon test assumes that the data without the suspected outlier (s) are normally distributed. If the user wants to perform a normality test on the data set, he should first remove the outliers before performing the normality test. This test tends to suffer from masking in the presence of multiple outliers. This means that if more than one outlier (in either tail) is suspected, this test may fail to identify all of the outliers.

Rosner Outlier Test: This test can be used to identify up to 10 outliers in data sets of sizes 25 and higher. This test also assumes that the data set without the suspected outliers is normally distributed. Like the Dixon test, if the user wants to perform a normality test on the data set, he should first remove the outliers (which are not known in advance) before performing the normality test. The detailed discussion of these two tests is given in the associated ProUCL Technical Guide. A couple of examples illustrating the identification of outliers in data sets with NDs are described in the following sections.

7.1 Outlier Test for Full Data Set

1. Click **Outlier Tests ► Full (w/o NDs) ► Compute**

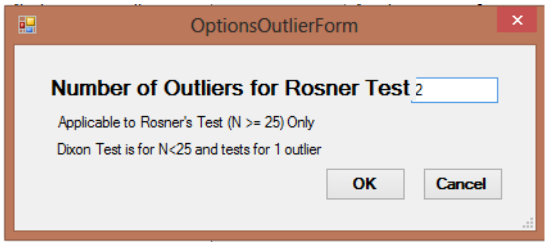


2. The **Select Variables** screen (Chapter 3) will appear.

- Select one or more variable(s) from the **Select Variables** screen.

- If outlier test needs to be performed by using a Group variable, then select a group variable by clicking the arrow below the **Select Group Column (Optional)** button. This will result in a drop-down list of available variables. The user should select and click on an appropriate variable representing a group variable.

- If at least one of the selected variables (or group) has 25 or more observations, then click the option button for the Rosner Test. ProUCL automatically performs the Dixon test for data sets of sizes ≤ 25.



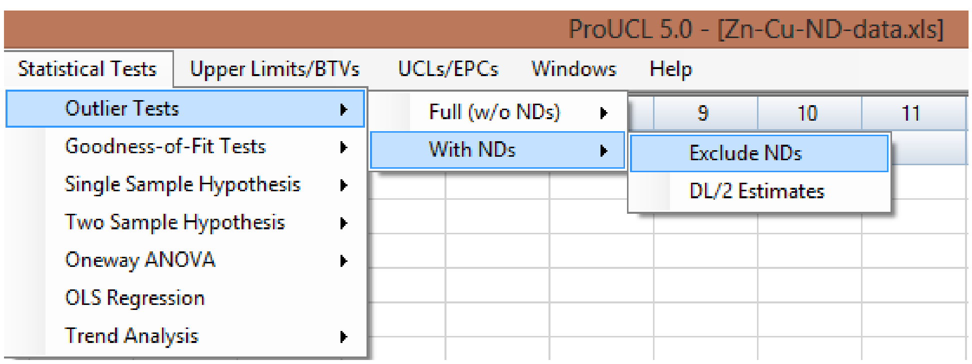
- The default option for the number of suspected outliers is 1. To use the Rosner test, the user has to obtain an initial guess about the number of suspected outliers that may be present in the data set. This can be done by using graphical displays such as a Q-Q plot. On a Q-Q plot, higher observations that are well separated from the rest of the data may be considered as potential or suspected outliers.

- Click on the **OK** button to continue or on the **Cancel** button to cancel the Outlier Test.

7.2 Outlier Test for Data Sets with NDs

Two options: exclude NDs; or replace NDs by their respective DL/2 are available in ProUCL to perform outlier tests on data sets with NDs.

1. Click **Outlier Tests ► With NDs ► Exclude NDs**



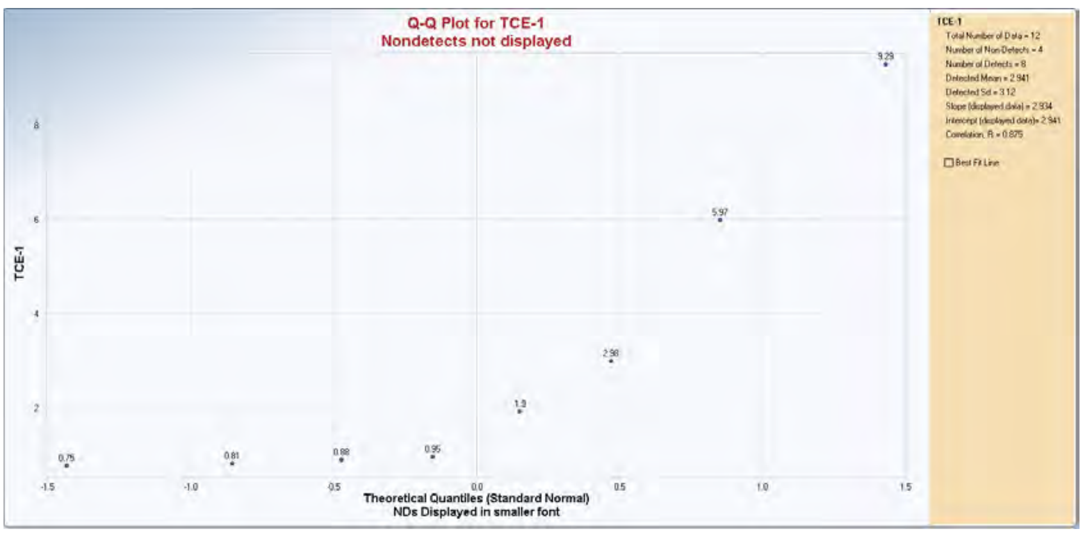
Note: The above screen shot was generated using ProUCL 5.0; the exactly similar screen is generated using ProUCL 5.1 with the exception that in the title of the screen shot, ProUCL 5.0 will be replaced by ProUCL 5.1. Therefore, to save time, many intermediate screen shots used in the ProUCL 5.0 User Guide have been used in this ProUCL 5.1 User Guide.

Output Screen for Dixon's Outlier Test

Dixon's Outlier Test for TCE-1
Total N = 12
Number NDs = 4
Number Detects = 8
10% critical value: 0.479
5% critical value: 0.554
1% critical value: 0.683
Note: NDs excluded from Outlier Test
1. Data Value 9.29 is a Potential Outlier (Upper Tail)?
Test Statistic: 0.392
For 10% significance level, 9.29 is not an outlier.
For 5% significance level, 9.29 is not an outlier.
For 1% significance level, 9.29 is not an outlier.

2. Data Value 0.75 is a Potential Outlier (Lower Tail)?
Test Statistic: 0.011
For 10% significance level, 0.75 is not an outlier.
For 5% significance level, 0.75 is not an outlier.
For 1% significance level, 0.75 is not an outlier.

Q-Q plot without Four Nondetect Observations are Shown as Follows



Example: Rosner's Outlier Test by a Group Variable, Zone

- Selected Options: Number of Suspected Outliers = 4
- NDs excluded from the Rosner Test
- Outlier test performed using the **Select Group Column (Optional)**

Output Screen for Rosner's Outlier Test for Zinc in Zone: Alluvial Fan

Rosner's Outlier Test for 4 Outliers in Zn (alluvial fan)

Total N	**67**
Number NDs	**16**
Number Detects	**51**
Mean of Detects	**27.88**
SD of Detects	**85.02**
Number of data	**51**
Number of suspected outliers	**4**
s not included in the following:	

#	Mean	sd	Potential outlier	Obs. Number	Test value	Critical value (5%)	Critical value (1%)
1	27.88	84.18	620	26	7.034	3.137	3.488
2	16.04	8.776	50	28	3.87	3.127	3.478
3	15.35	7.356	40	27	3.352	3.118	3.469
4	14.83	6.485	33	29	2.801	3.108	3.468

For 5% significance level, there are 3 Potential Outliers

620, 50, 40

For 1% Significance Level, there are 2 Potential Outliers

620, 50

Q-Q plot for Zinc Based upon Detected Data (Alluvial Fan)

Output Screen for Rosner's Outlier Test for Zinc in Zone: Basin Trough

Rosner's Outlier Test for 4 Outliers in Zn (basin trough)

Total N	**50**
Number NDs	**4**
Number Detects	**46**
Mean of Detects	**23.13**
SD of Detects	**19.03**
Number of data	**46**
Number of suspected outliers	**4**
s not included in the following:	

#	Mean	sd	Potential outlier	Obs. Number	Test value	Critical value (5%)	Critical value (1%)
1	23.13	18.82	90	45	3.553	3.09	3.45
2	21.64	16.32	70	21	2.963	3.09	3.44
3	20.55	14.73	60	3	2.679	3.08	3.43
4	19.63	13.57	60	22	2.975	2.07	3.41

For 5% significance level, there are 4 Potential Outliers

90, 70, 60, 60

For 1% Significance Level, there is 1 Potential Outlier

Chapter 8

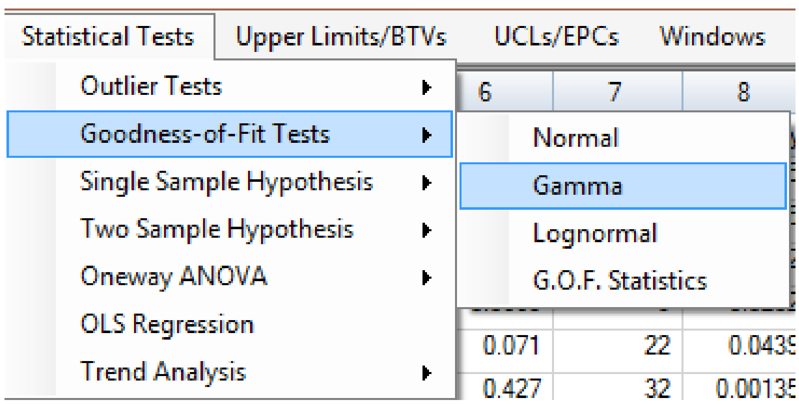
Goodness-of-Fit (GOF) Tests for Uncensored and Left-Censored Data Sets

GOF tests are available under the **Statistical Test** module of ProUCL 5.0/ProUCL 5.1. Throughout this User Guide and in ProUCL software, "Full" represents uncensored data sets without ND observations. The details and usage of the various GOF tests are described in the associated ProUCL Technical Guide. In ProUCL 5.1, critical values associated with Lilliefors normality test are computed using a more efficient algorithm as described in the associated ProUCL 5.1 Technical Guide. Therefore, tables and graphs involving Lilliefors test have been re-generated using ProUCL 5.1.

8.1 Goodness-of-Fit Test in ProUCL

Several GOF tests for uncensored full (**Full (w/o NDs)**) and left-censored (**With NDs**) data sets are available in the ProUCL software.

- **Full (w/o NDs)**



  - This option is used on uncensored full data sets without any ND observations. This option can be used to determine GOF for normal, gamma, or lognormal distribution of the variable(s) selected using the **Select Variables** option.

  - Like all other methods in ProUCL, GOF tests can also be performed on variables categorized by a Group ID variable.

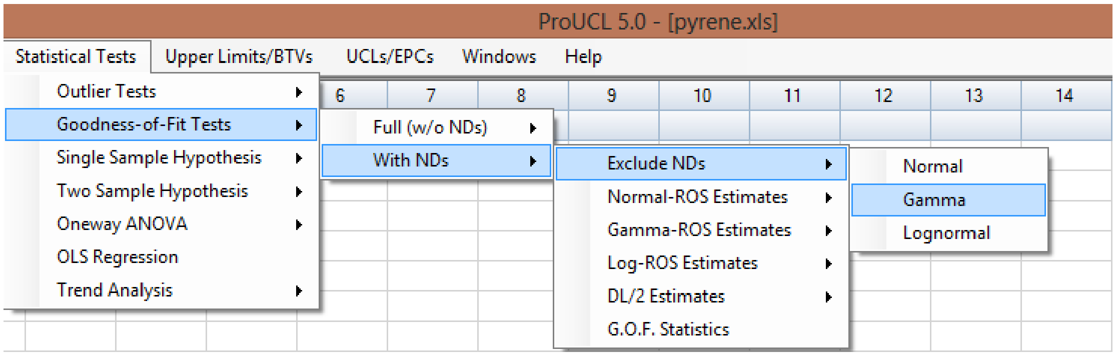
  - Based upon the hypothesized distribution (normal, gamma, lognormal), a Q-Q plot displaying all statistics of interest including the derived conclusion is also generated.

  - The **G.O.F. Statistics** option generates a detailed output log (Excel type spreadsheet) showing all GOF test statistics (with derived conclusions) available in ProUCL. This option helps a user to determine the distribution of a data set before generating a GOF Q-Q plot for the hypothesized distribution. This option was included at the request of some users in earlier versions of ProUCL.

- **With NDs**

  - This option performs GOF tests on data sets consisting of both nondetected and detected data values.

  - Several sub-menu items shown below are available for this option.



1. **Exclude NDs**: tests for normal, gamma, or lognormal distribution of the selected variable(s) using only the detected values.

2. **ROS Estimates**: tests for normal, gamma, or lognormal distribution of the selected variable(s) using detected values and imputed nondetects.

   - Three ROS methods for normal, lognormal (Log), and gamma distributions are available. This option imputes the NDs based upon the specified distribution and performs the specified GOF test on the data set consisting of detects and imputed nondetects.

3. **DL/2 Estimates**: tests for normal, gamma, or lognormal distribution of the selected variable(s) using the detected values and the ND values replaced by their respective DL/2 values. This option is included for historical reasons and also for curious users. ProUCL does not make any recommendations based upon this option.

4. **G.O.F. Statistics:** Like full uncensored data sets, this option generates an output log of all GOF test statistics available in ProUCL for data sets with nondetects. The conclusions about the data distributions for all selected variables are also displayed on the generated output file (Excel-type spreadsheet).

- **Multiple variables:** When multiple variables are selected from the **Select Variables** screen, one can use one of the following two options:

  - Use the **Group Graph**s option to produce multiple GOF Q-Q plots for all selected variables in a single graph. This option may be used when a selected variable has data coming from two or more groups or populations. The relevant statistics (e.g., slope, intercept, correlation, test statistic and critical value) associated with the selected variables are shown on the right panel of the GOF Q-Q plot. To capture all the graphs and results shown on the window screen, it is preferable to print the graph using the

Landscape option. The user may also want to turn off the Navigation Panel and Log Panel.

  - The **Individual Graphs** option is used to generate individual GOF Q-Q plots for each of the selected variables, one variable at a time (or for each group individually of the selected variable categorized by a Group ID). This is the most commonly used option to perform GOF tests for the selected variables.

- **GOF Q-Q plots for hypothesized distributions:** ProUCL computes the relevant test statistic and the associated critical value, and prints them on the associated Q-Q plot (called GOF Q-Q plot). On a GOF Q-Q plot, the program informs the user if the data are gamma, normally, or lognormally distributed.

  - For all options described above, ProUCL generates GOF Q-Q plots based upon the hypothesized distribution (normal, gamma, lognormal). All GOF Q-Q plots display several statistics of interest including the derived conclusion.

  - The linear pattern displayed by a GOF Q-Q plot suggests an approximate GOF for the selected distribution. The program computes the intercept, slope, and the correlation coefficient for the linear pattern displayed by the Q-Q plot. A high value of the correlation coefficient (e.g., > 0.95) may be an indication of a good fit for that distribution; however, the high correlation should exhibit a definite linear pattern in the Q-Q plot without breaks and discontinuities.

  - On a GOF Q-Q plot, observations that are well separated from the majority of the data typically represent potential outliers needing further investigation.

  - Significant and obvious jumps and breaks and curves in a Q-Q plot are indications of the presence of more than one population. Data sets exhibiting such behavior of Q-Q plots may require partitioning of the data set into component subsets (representing sub-populations present in a mixture data set) before computing upper limits to estimate EPCs or BTVs. It is recommended that both graphical and formal goodness-of-fit tests be used on the same data set to determine the distribution of the data set under study.

- **Normality or Lognormality Tests**: In addition to informal graphical normal and lognormal Q-Q plots, a formal GOF test is also available to test the normality or lognormality of the data set.

  - Lilliefors Test: a test typically used for samples of size larger than 50 (> 50). However, the Lilliefors test (generalized Kolmogorov Smirnov [KS] test) is available for samples of all sizes. There is no applicable upper limit for sample size for the Lilliefors test.

  - Shapiro and Wilk (SW, S-W) Test: a test used for samples of size smaller than or equal to 2000 (<= 2000). In ProUCL 5.0, the SW test uses the exact SW critical values for samples of size 50 or less. For samples of size, greater than 50, the SW test statistic is displayed along with the *p*-value of the test (Royston 1982, 1982a).

Notes: As with other statistical tests, sometimes these two GOF tests might lead to different conclusions. The user is advised to exercise caution when interpreting these test results. When one the GOF tests passes the hypothesized distribution, ProUCL 5.0/ProUCL 5.1 determines that the data set follows an approximate hypothesized distribution. It should be pointed out that for data sets of smaller sizes (e.g., <50), when Lilliefors tests determines that the data set follows a normal (lognormal) distribution and Shapiro-Wilk's test determines that the data set does not follow a normal (lognormal) distribution, the user may not use the approximate normality (lognormality) conclusion derived using the Lilliefors test. Under these situations, the user may determine the data distribution based upon the highest p-value associated with GOF test statistics for other distributions or may determine that the data set does not follow a discernible distribution.

- **GOF test for Gamma Distribution:** In addition to the graphical gamma Q-Q plot, two formal empirical distribution function (EDF) procedures are also available to test the gamma distribution of a data set. These tests are the AD test and the KS test.

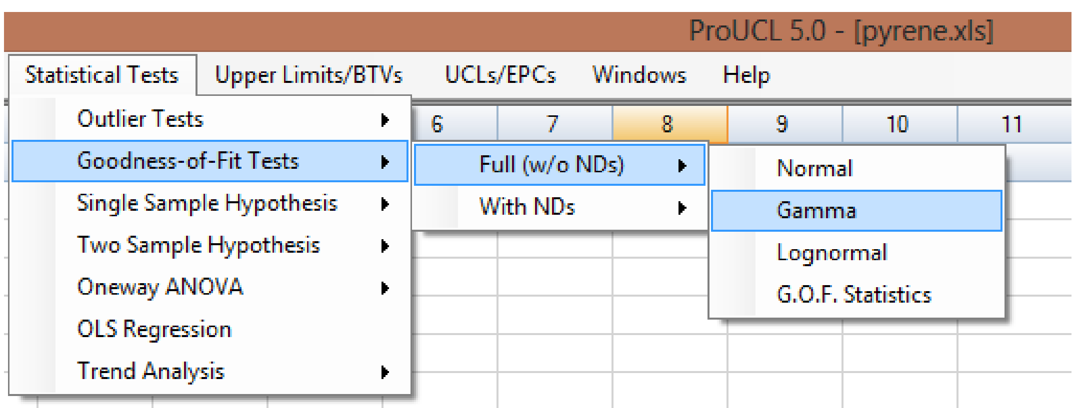
  - It is noted that these two tests might lead to different conclusions. Therefore, the user should exercise caution interpreting the results.

  - These two tests may be used for samples of sizes in the range of 4 - 2500. Also, for these two tests, the value (known or estimated) of the shape parameter, *k* (*k* hat) should lie in the interval [0.01, 100.0]. Consult the associated ProUCL Technical Guide for a detailed description of the gamma distribution and its parameters, including *k*. Extrapolation of critical values beyond these sample sizes and values of *k* is not recommended.

  Notes: Even though, the **GOF Statistics** option prints out all GOF test statistics for all selected variables, it is suggested that the user should look at the graphical Q-Q plot displays to gain extra insight (e.g., outliers, multiple population) into the data set.

8.2 Goodness-of-Fit Tests for Uncensored Full Data Sets

1. Click **Goodness-of-Fit Tests ► Full (w/o NDs)**



2. Select the distribution to be tested: Normal, Lognormal, or Gamma

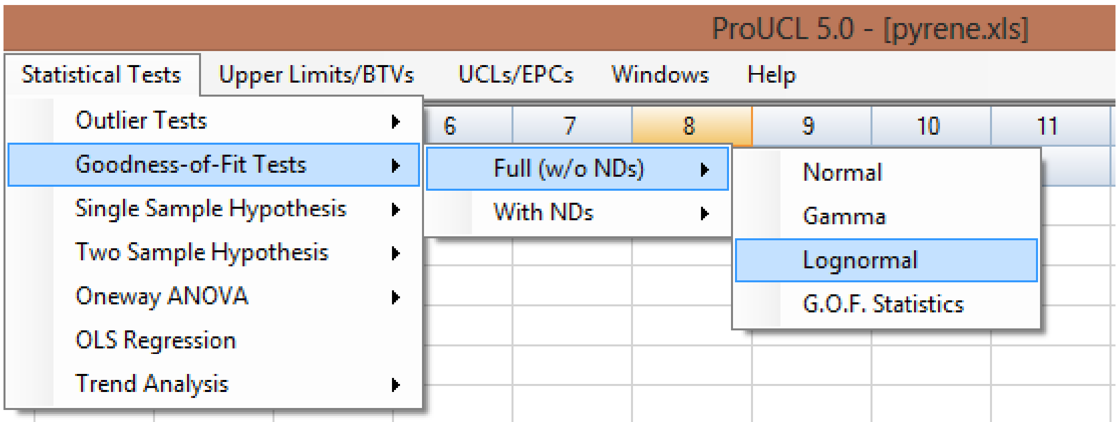
   - To test for normality, click on **Normal** from the drop-down menu list.

   - To test for lognormality, click on **Lognormal** from the drop-down menu list.

   - To test for gamma distribution, click on **Gamma** from the drop-down menu list.

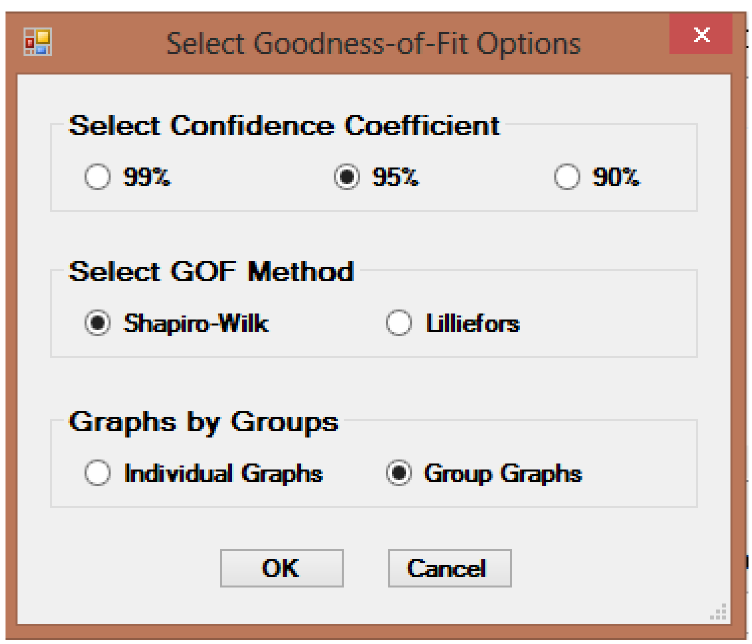
8.2.1 GOF Tests for Normal and Lognormal Distribution

1. Click **Goodness-of-Fit Tests ► Full (w/o NDs) ► Normal or Lognormal**



2. The **Select Variables** screen (Chapter 3) will appear.

- Select one or more variable(s) from the **Select Variables** screen.
- If graphs have to be produced by using a Group variable, then select a group variable by clicking the arrow below the **Select Group Column (Optional)** button. This will result in a drop-down list of available variables. The user should select and click on an appropriate variable representing a group variable.
- When the **Option** button is clicked, the following window will be shown.



  - The default option for the **Confidence Level** is **95%**.

- The default GOF Method is **Shapiro-Wilk**.

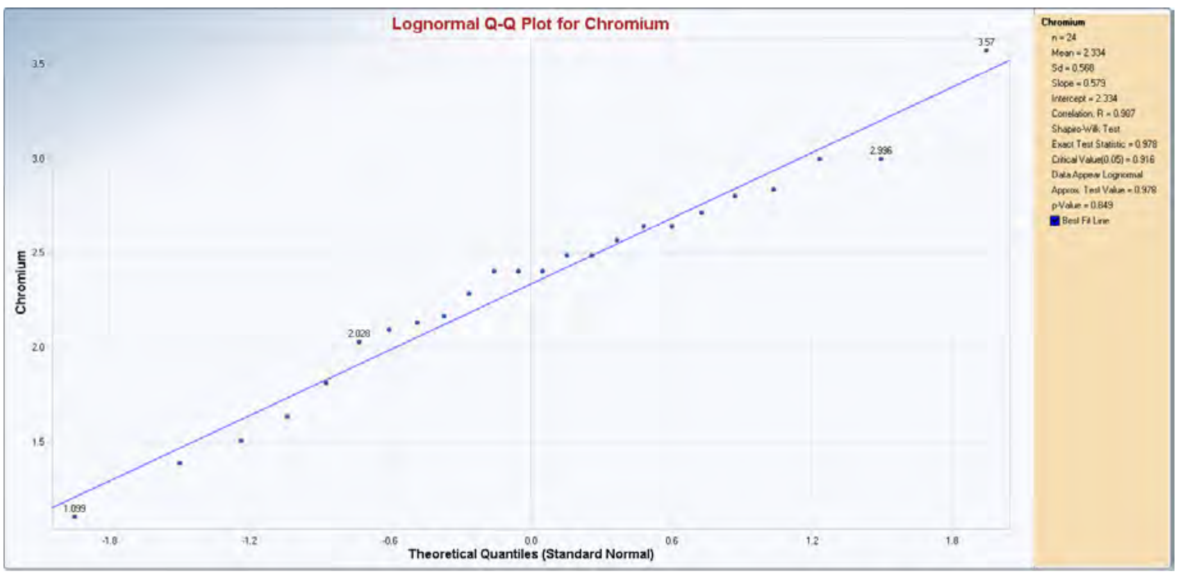
- The default option for **Graphs by Group** is **Group Graphs**. If you want to see the plots for all selected variables individually, and then check the button next to **Individual Graphs**.

- Click **OK** button to continue or **Cancel** button to cancel the GOF tests.

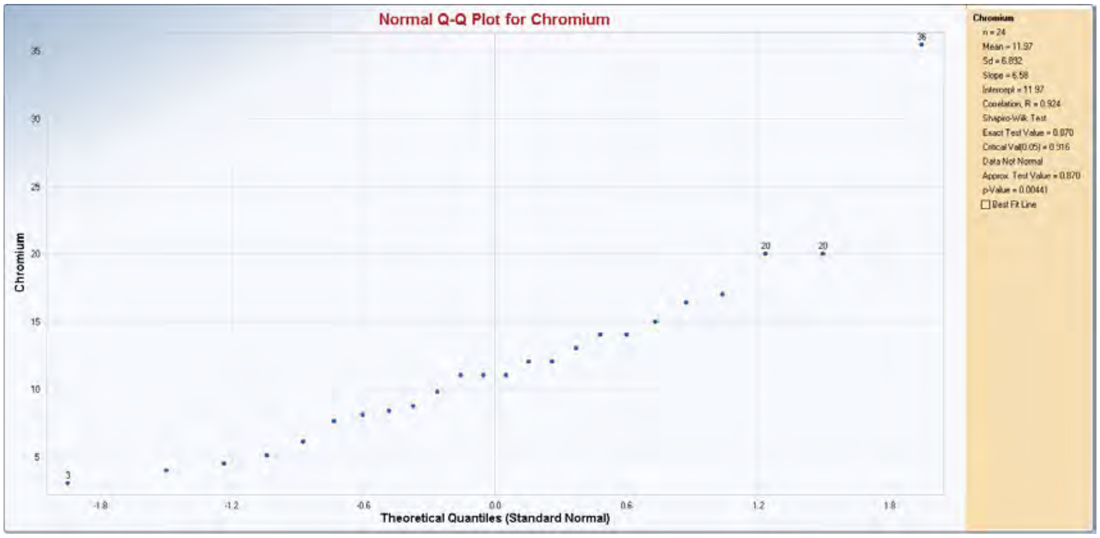
<u>Notes</u>: This option for **Graphs by Group** is specifically provided for when the user wants to display multiple graphs for a variable by a group variable (e.g., site AOC1, site AOC2, background). This kind of display represents a useful visual comparison of the values of a variable (e.g., concentrations of COPC-Arsenic) collected from two or more groups (e.g., upgradient wells, monitoring wells, residential wells).

Example 8-1a Consider the chromium concentrations data set used in Example 1-1 of Chapter 1. The lognormal and normal GOF test results on chromium concentrations are shown in the following figures.

Output Screen for Lognormal Distribution (Full (w/o NDs))
Selected Options: Shapiro-Wilk

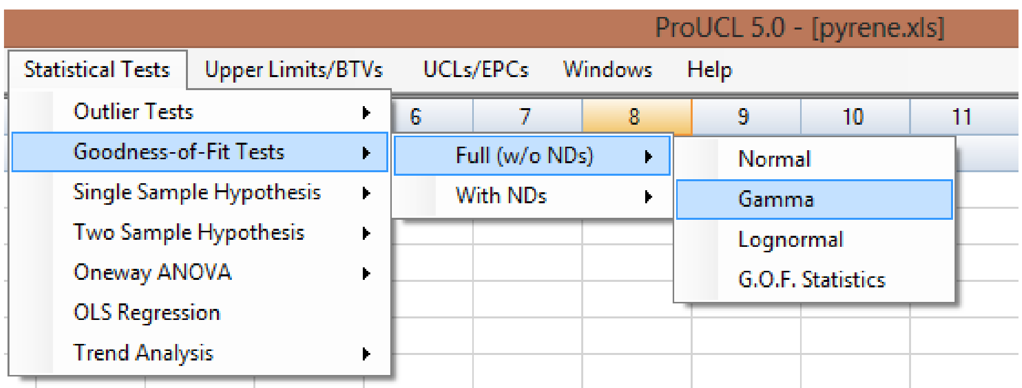


Output Screen for Normal Distribution (Full (w/o NDs))
Selected Options: Shapiro-Wilk, Best Fit Line not Displayed



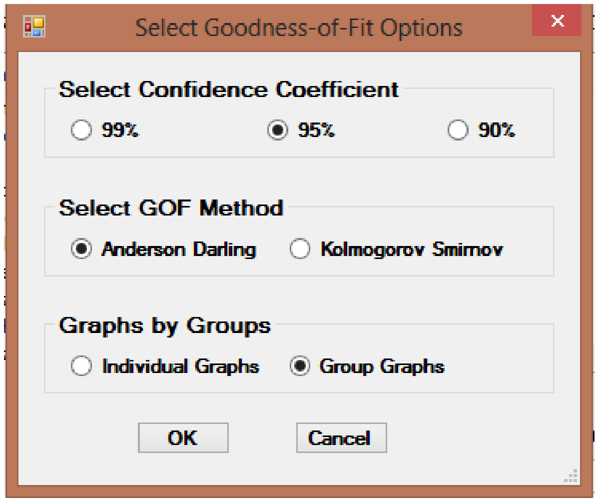
8.2.2 GOF Tests for Gamma Distribution

1. Click **Goodness-of-Fit Tests ► Full (w/o NDs) ► Gamma**



2. The **Select Variables** screen (described in Chapter 3) will appear.

- Select one or more variable(s) from the **Select Variables** screen.
- If graphs have to be produced by using a group variable, then select a group variable by clicking the arrow below the **Select Group Column (Optional)** button. This will result in a drop-down list of available variables. The user should select and click on an appropriate variable representing a group variable.
- When the option button is clicked, the following window will be shown.



- The default option for the **Confidence Coefficient** is **95%**.

- The default GOF method is **Anderson Darling**.

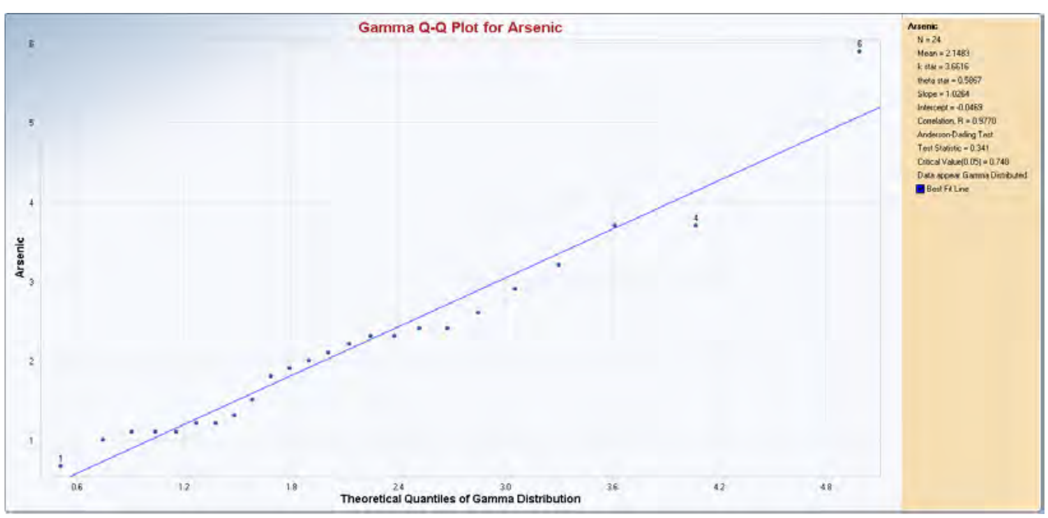
- The default option for **Graph by Groups** is **Group Graphs**. If you want to see individual graphs, then check the radio button next to **Individual Graphs**.

- Click the **OK** button to continue or the **Cancel** button to cancel the option.

- Click **OK** button to continue or **Cancel** button to cancel the GOF tests.

Example 8-1b. Consider arsenic concentrations data set used in Example 1-1 of Chapter 1. The Gamma GOF test results for arsenic concentrations, are shown in the following G.O.F. Q-Q plot.

Output Screen for Gamma Distribution (Full (w/o NDs))
Selected Options: Anderson Darling with Best Line Fit



8.3 Goodness-of-Fit Tests Excluding NDs

This option is the most important option for a GOF test applied to data sets with ND observations. Based upon the skewness and distribution of detected data, ProUCL computes the appropriate decision statistics (UCLs, UPLs, UTLs, and USLs) which accommodate data skewness. Specifically, depending upon the distribution of detected data, ProUCL uses KM estimates in parametric or nonparametric upper limits computation formulae (UCLs, UTLs) to estimate EPC and BTV estimates.

1. Click **Goodness-of-Fit Tests ► With NDs ► Exclude NDs**

2. Select distribution to be tested: Normal, Gamma, or Lognormal.

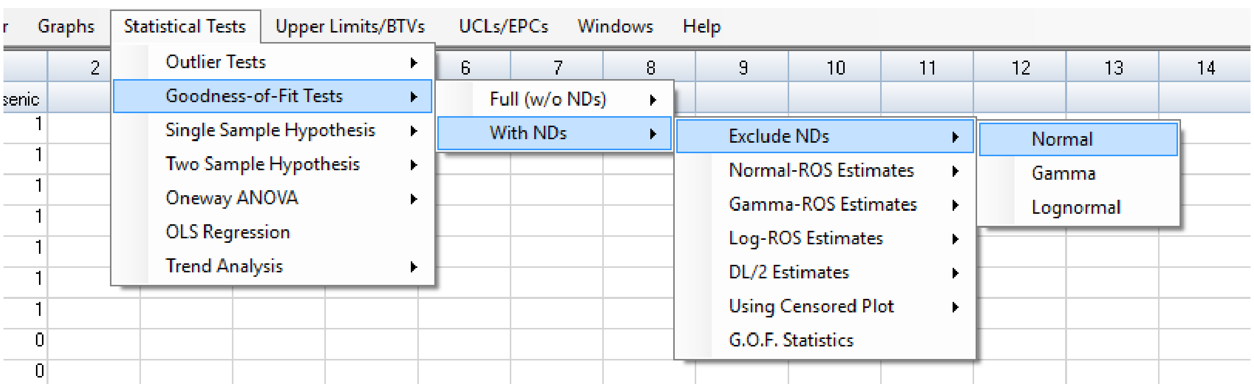
   - To test for normality, click on **Normal** from the drop-down menu list.

   - To test for lognormality, click on **Lognormal** from the drop-down menu list.

   - To test for gamma distribution, click on **Gamma** from the drop-down menu list.

8.3.1 Normal and Lognormal Options

1. Click **Goodness-of-Fit Tests ► With NDs ►Excluded NDs ► Normal or Lognormal**



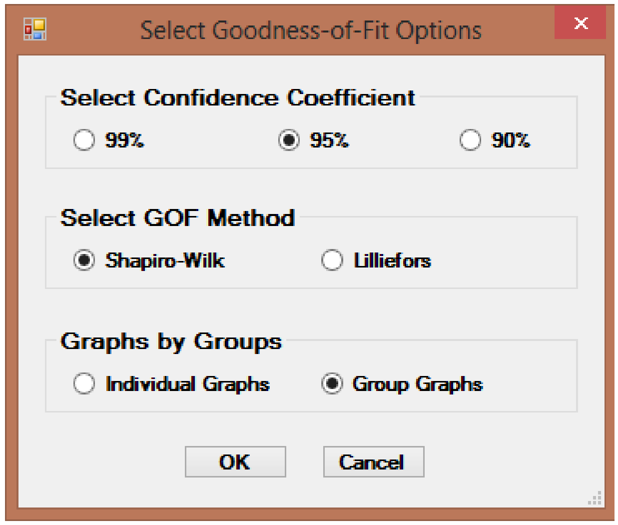
Note: In ProUCL 5.1, the censored probability plot option has been added as shown in the above drop-down menu as "**Using Censored Plot**." This option is very much the same as the Q-Q plot option generated by excluding NDs except that the hypothesized quantiles displayed along the x-axis adjust for quantiles associated with NDs. There is not much difference (except for the correlation, slope and intercept of the optional line displayed on the Q-Q plot) between these two graphs from the decision making point of view. Censored probability (Q-Q) plots do not provide additional information than tools and graphs already available in ProUCL 5.0. This was the reason that censored Q-Q plots were not included in ProUCL 5.0 and its earlier versions.

2. The **Select Variables** screen (Chapter 3) will appear.

   - Select one or more variable(s) from the **Select Variables** screen.

- If graphs have to be produced by using a group variable, then select a group variable by clicking the arrow below the **Select Group Column (Optional)** button. This will result in a drop-down list of available variables. The user should select and click on an appropriate variable representing a group variable.

- When the option button: **Normal** or **Lognormal** is clicked, following window appears.



  - The default option for the **Confidence Coefficient** is **95%**.

  - The default GOF Method is **Shapiro-Wilk**.

  - The default option for **Graphs by Group** is **Group Graphs**. If you want to see the plots for all selected variables individually, then check the button next to **Individual Graphs**.

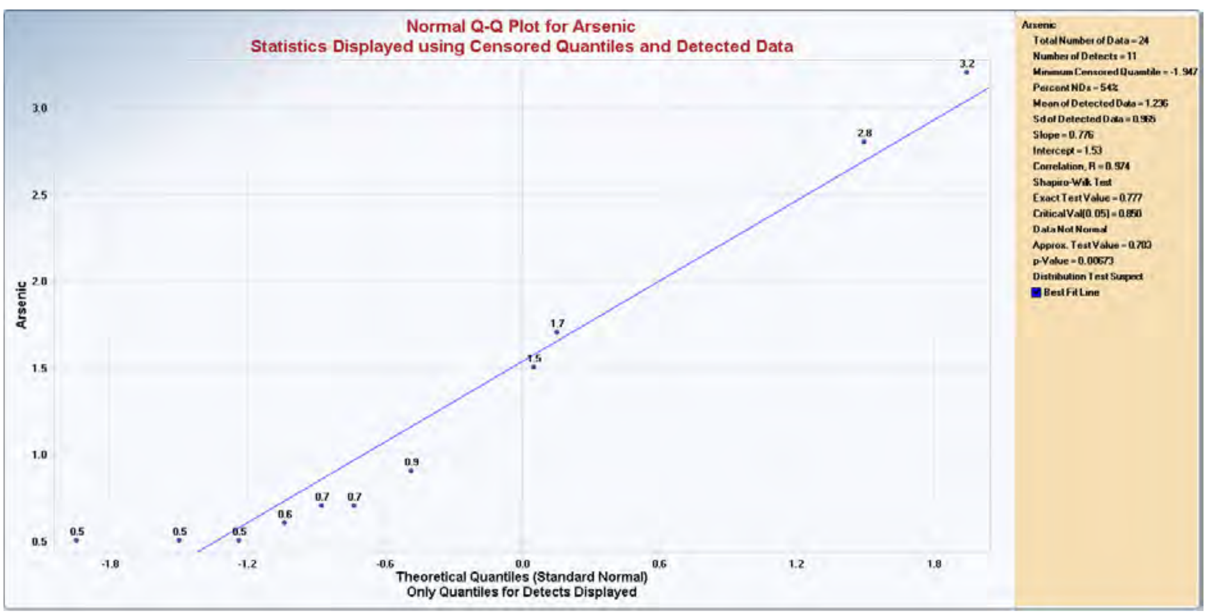
- Click the **OK** button to continue or the **Cancel** button to cancel the option.

- Click the **OK** button to continue or the **Cancel button** to cancel the GOF tests.

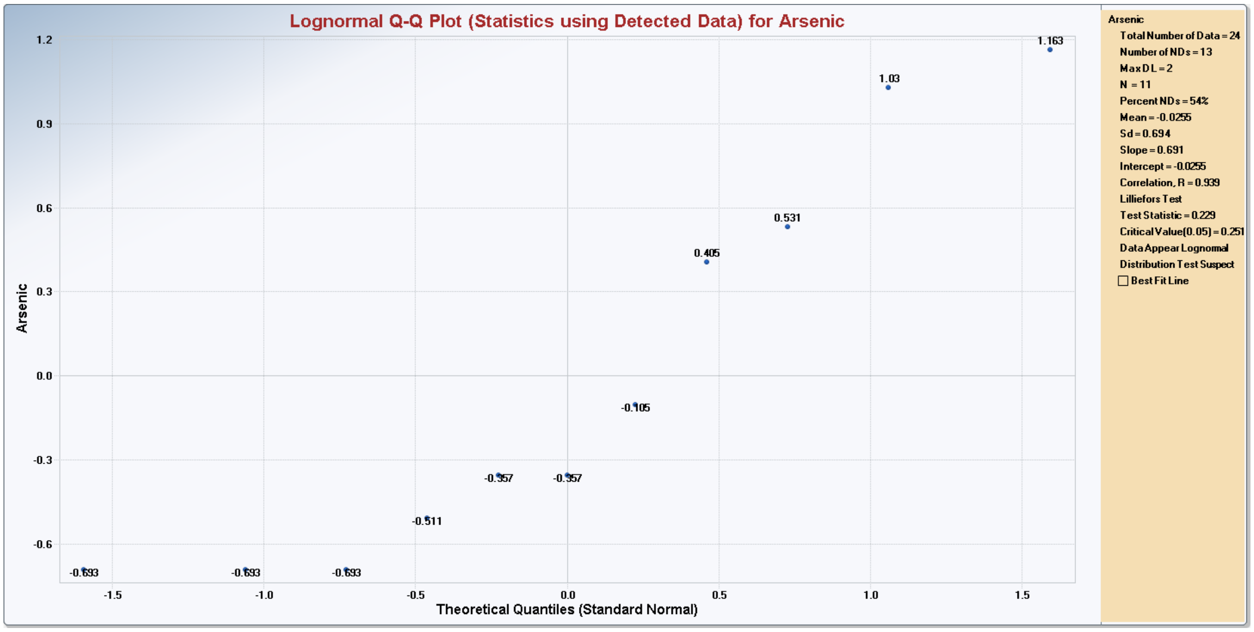
Example 8-2a. Consider the arsenic Oahu data set with NDs discussed in the literature (e.g., Helsel 2012; NADA in R [Helsel 2013]). The normal and lognormal GOF test results based upon the detected data are shown in the following two figures. Censored Q-Q plots are also displayed along with Q-Q plots based upon detected data.

GOF Q-Q Plot for Normal Distribution (Exclude NDs)
Selected Options: Shapiro-Wilk

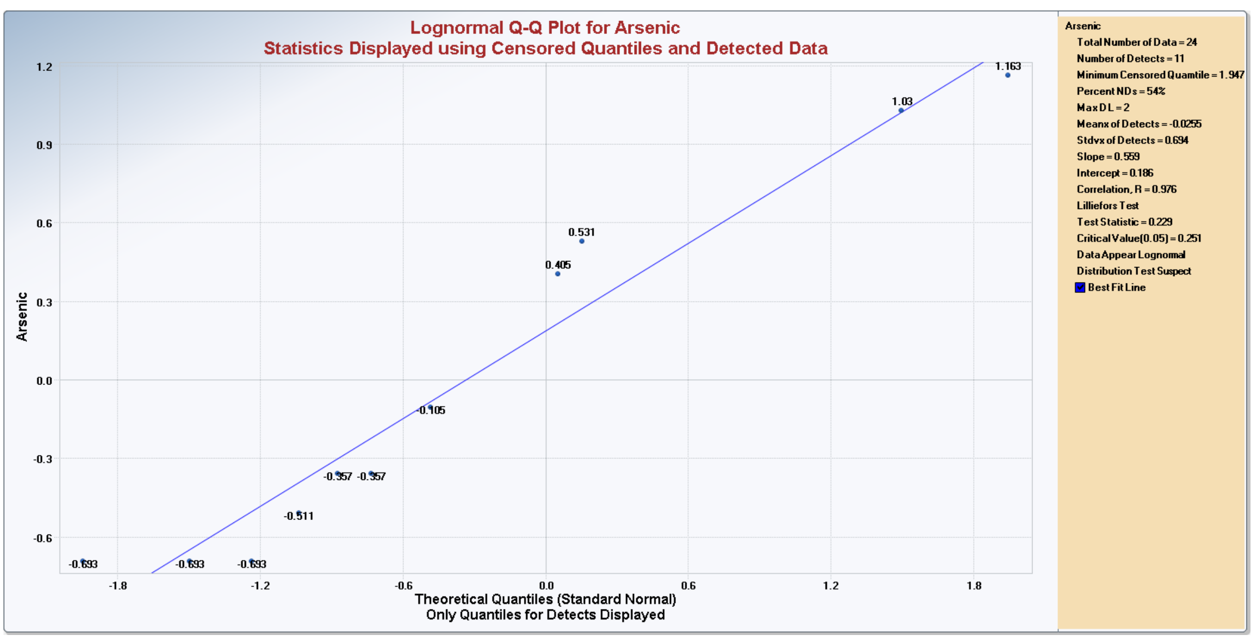
Censored Probability (Q-Q) Plot for Normal Distribution
Selected Options: Shapiro-Wilk and Best Line Fit



GOF Q-Q Plot for Lognormal Distribution (Exclude NDs)
Selected Options: Lilliefors Test

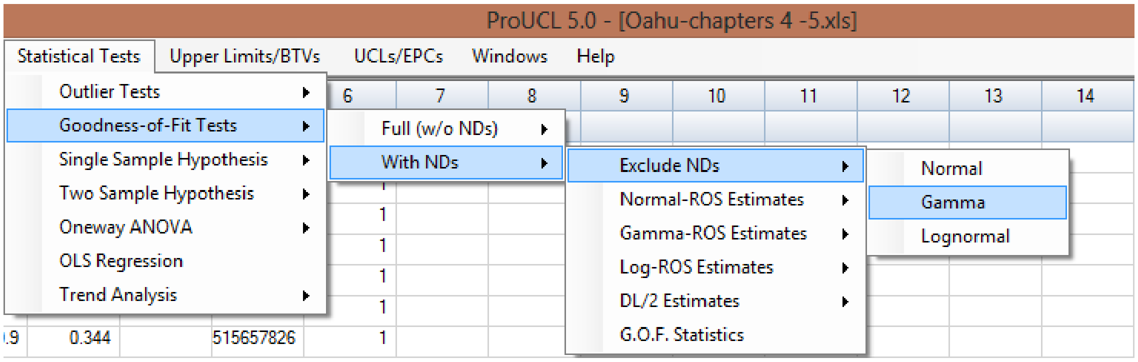


Censored Probability (Q-Q) Plot for Lognormal Distribution
Selected options: Lilliefors Test with Best Fit Line



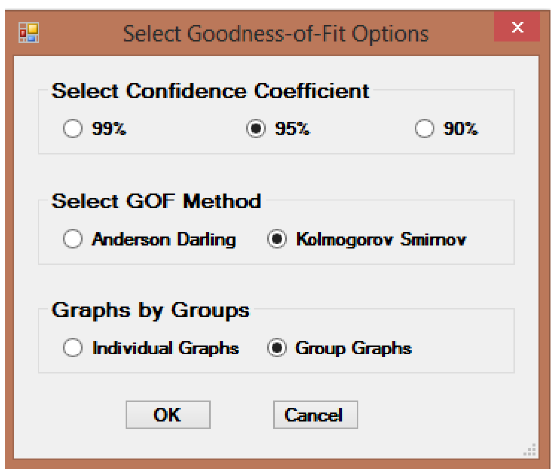
8.3.2 Gamma Distribution Option

1. Click **Goodness-of-Fit Tests ► With NDs ► Excluded NDs ► Gamma**



2. The **Select Variables** screen (Chapter 3) will appear.

- Select one or more variable(s) from the **Select Variables** screen.
- If graphs have to be produced by using a Group variable, then select a group variable by clicking the arrow below the **Select Group Column (Optional)** button. This will result in a drop-down list of available variables. The user should select and click on an appropriate variable representing a group variable.
- When the option button (**Gamma**) is clicked, the following window is shown.



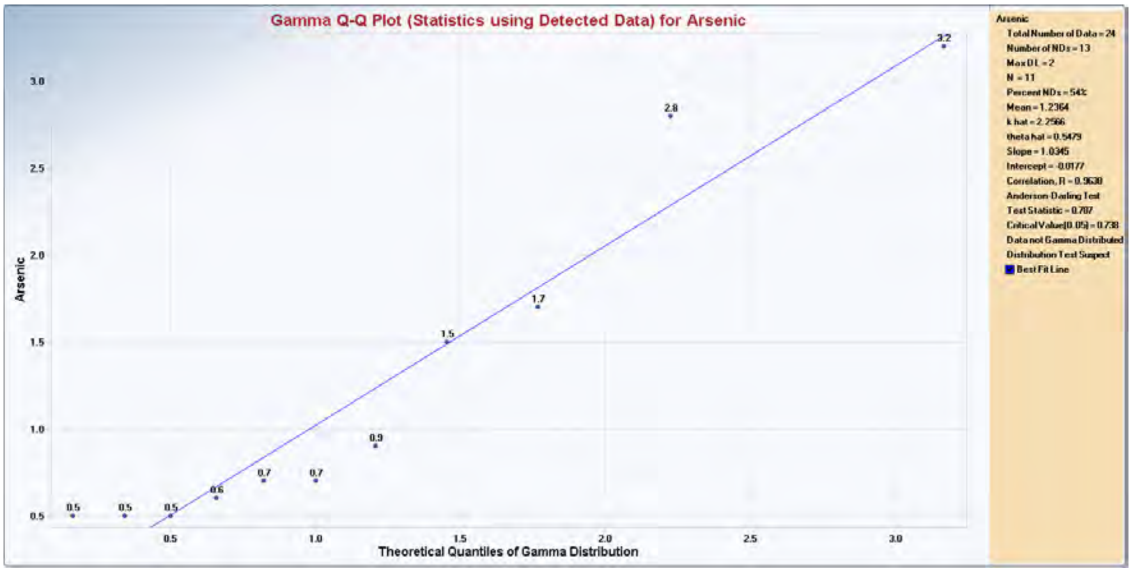
  - The default option for the **Confidence Coefficient** is **95%**.
  - The default GOF test method is the **Anderson Darling test**.
  - The default option for **Graph by Groups** is **Groups Graphs**. If you want to display all selected variables on separate graphs, check the button next to **Individual Graphs**.

- Click the **OK** button to continue or the **Cancel** button to cancel the option.

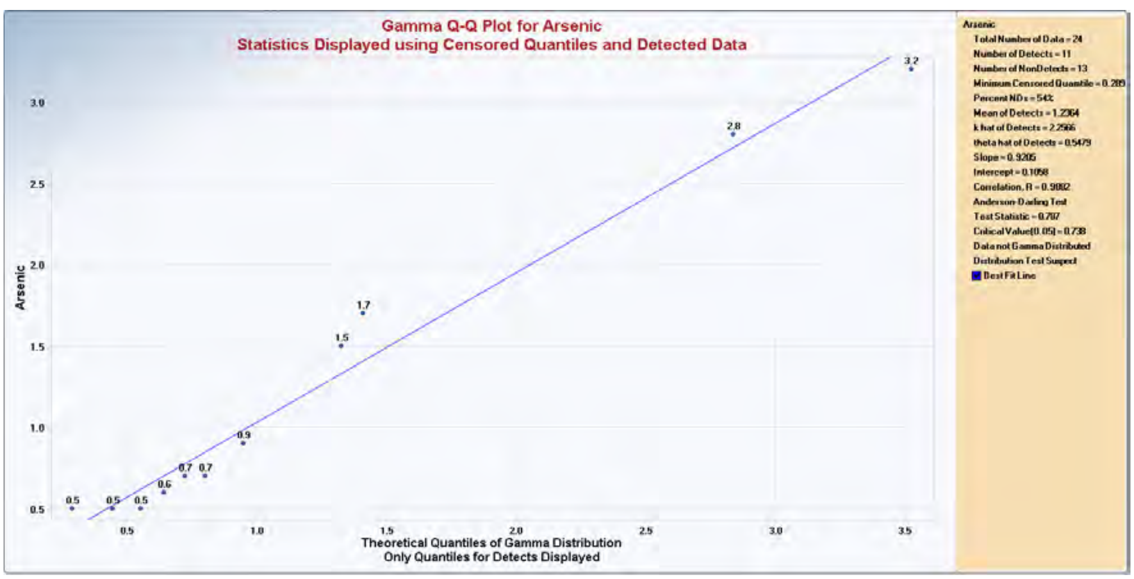
- Click the **OK** button to continue or the **Cancel** button to cancel the GOF tests.

Example 8-2b (continued). Consider the arsenic Oahu data set with NDs as discussed in Example 8-2a above. The gamma GOF test results based upon the detected data are shown in the following GOF Q-Q plot.

Output Screen for Gamma Distribution (Exclude NDs)
Selected Options: Anderson-Darling Test with Best Fit Line

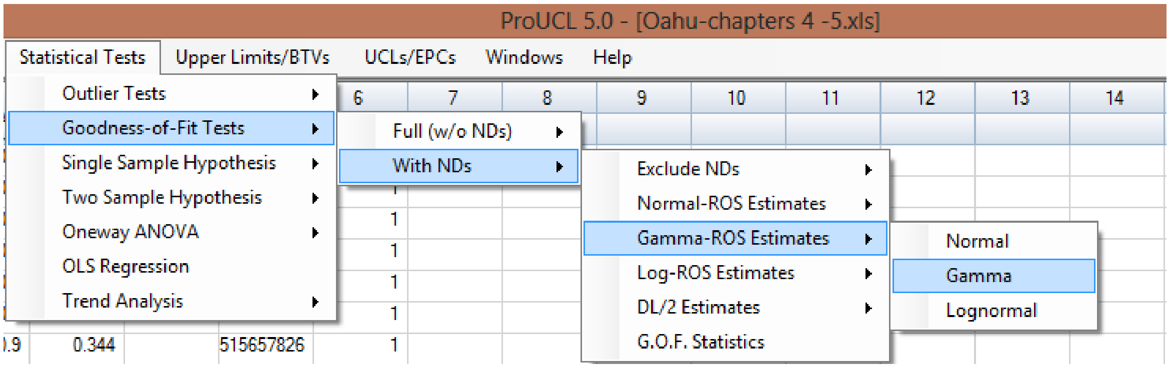


Censored Probability (Q-Q) Plot for Gamma Distribution
Selected options: Anderson-Darling Test with Best Fit Line



8.4 Goodness-of-Fit Tests with ROS Methods

1. Click **Goodness-of-Fit Tests ► With NDs ► Gamma-ROS Estimates or Log-ROS Estimates**

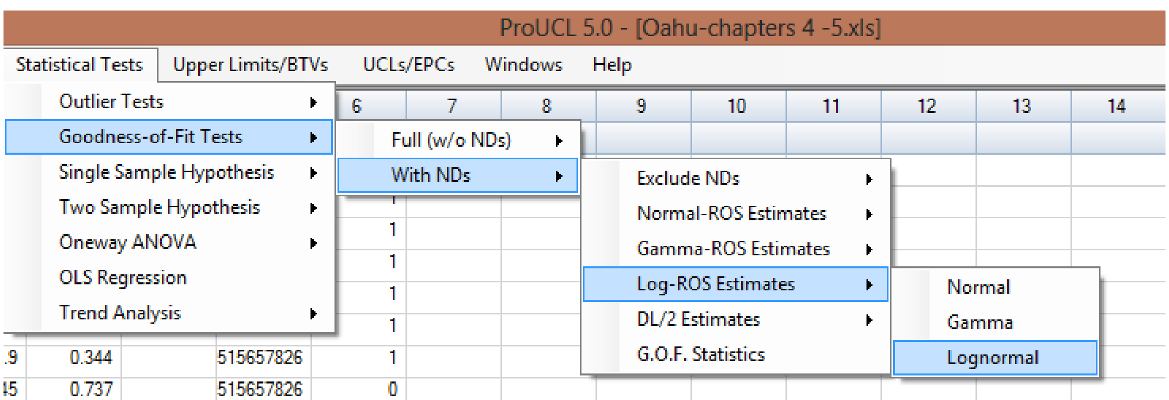


2. Select the distribution to be tested: Normal, Lognormal, or Gamma

- To test for normal distribution, click on **Normal** from the drop-down menu list.
- To test for gamma distribution, click on **Gamma** from the drop-down menu list.
- To test for lognormal distribution, click on **Lognormal** from the drop-down menu.

8.4.1 Normal or Lognormal Distribution (Log-ROS Estimates)

1. Click **Goodness-of-Fit Tests ► With NDs ► Log-ROS Estimates ► Normal, Lognormal**

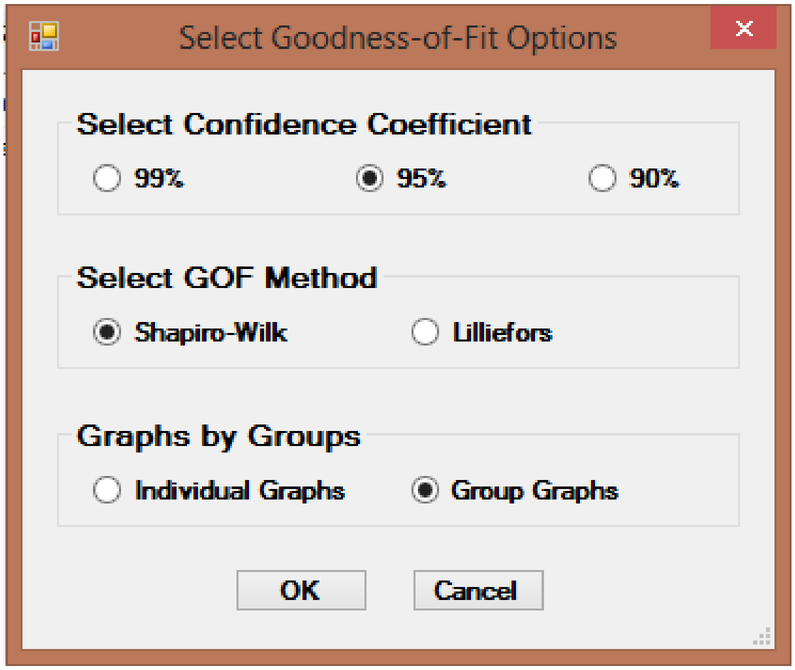


2. The **Select Variables** screen (Chapter 3) will appear.

- Select one or more variable(s) from the **Select Variables** screen.
- If graphs have to be produced by using a group variable, then select a group variable by clicking the arrow below the **Select Group Column (Optional)** button. This will result

in a drop-down list of available variables. The user should select and click on an appropriate variable representing a group variable.

- When the option button: Normal or Lognormal is clicked, the following window appears.



  - The default option for the **Confidence Coefficient** is **95%**.

  - The default GOF test Method is **Shapiro-Wilk**.

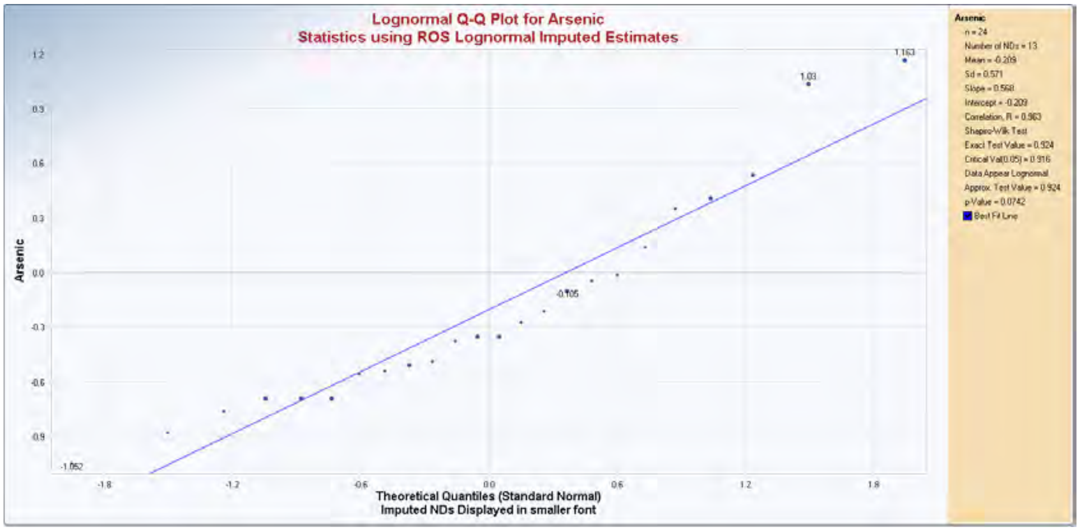
  - The default option for **Graphs by Group** is **Group Graphs**. If you want to display graphs for all selected variables individually, check the button next to **Individual Graphs**.

- Click the **OK** button to continue or the **Cancel** button to cancel the option.

- Click the **OK** button to continue or the **Cancel** button to cancel the GOF tests.

Example 8-2c (continued). Consider the arsenic Oahu data set with NDs considered earlier in this chapter. The lognormal GOF test results on LROS data (detected and imputed LROS NDs) is shown in the following GOF Q-Q plot.

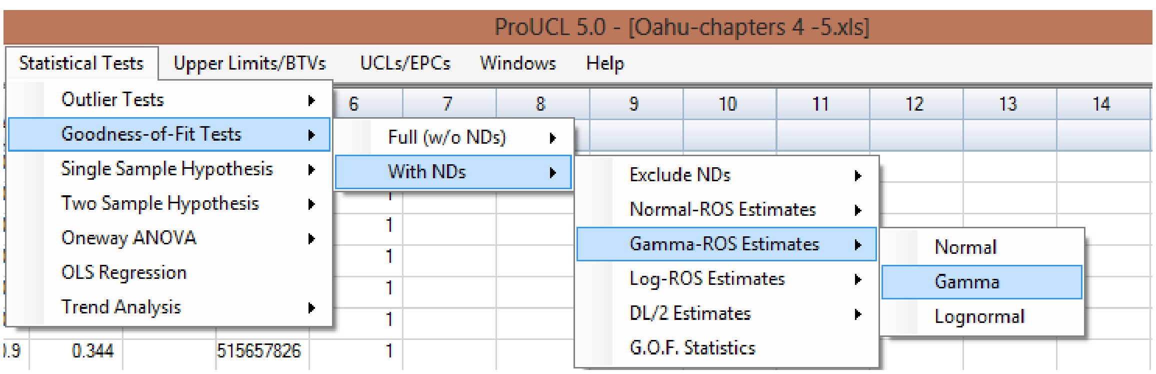
Output Screen for Lognormal Distribution (Log-ROS Estimates)
Selected Options: Shapiro Wilk test with Best Line Fit



Note**:** The font size of ND values is smaller than that of the detected values.

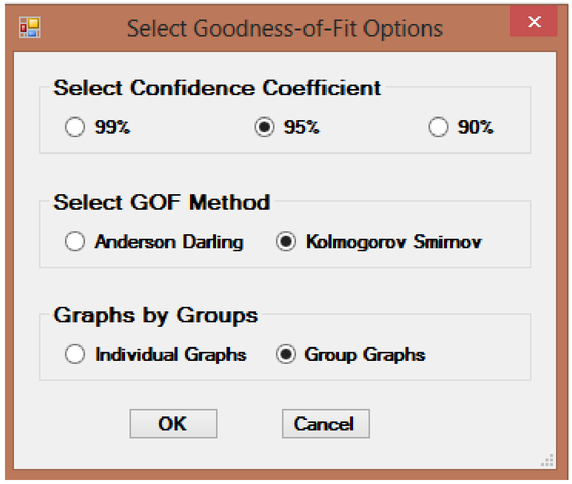
8.4.2 Gamma Distribution (Gamma-ROS Estimates)

1. Click **Goodness-of-Fit Tests ► With NDs ► Gamma-ROS Estimates ► Gamma**



2. The **Select Variables** screen (Chapter 3) will appear.

- Select one or more variable(s) from the **Select Variables** screen.
- If graphs have to be generated by using a Group variable, then select a group variable by clicking the arrow below the **Select Group Column (Optional)** button. This will result in a drop-down list of available variables. The user should select and click on an appropriate variable representing a group variable.
- When the option button (**Gamma**) is clicked, the following window will be shown.

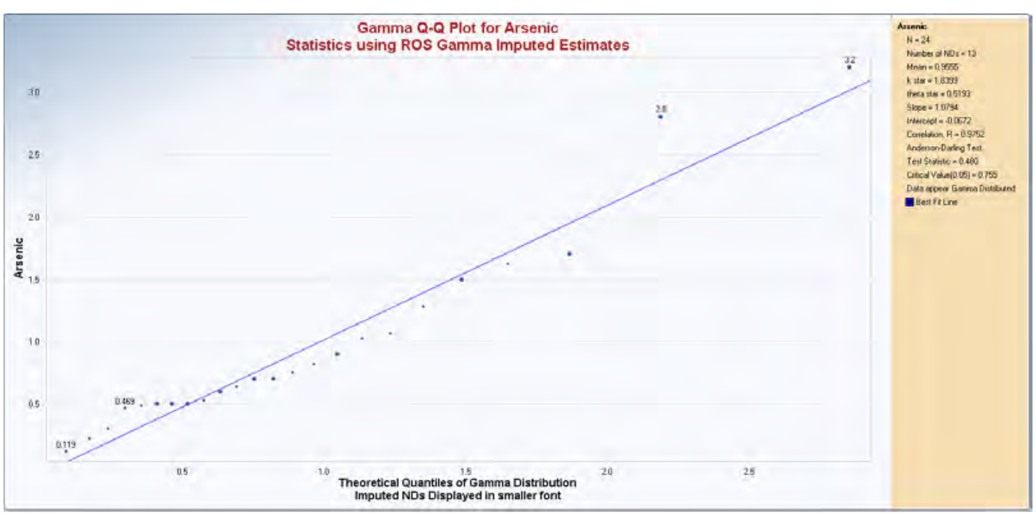


- o The default option for the **Confidence Coefficient** is **95%**.
- o The default GOF test **Method** is **Anderson Darling**.
- o The default option for **Graph by Groups** is Group **Graphs**. If you want to generate separate graphs for all selected variables, the check the button next to **Individual Graphs**.

- Click the **OK** button to continue or the **Cancel** button to cancel the GOF tests.

Example 8-2d (continued). Consider the arsenic Oahu data set with NDs considered earlier. The gamma GOF test results on GROS data (detected and imputed GROS NDs) are shown in the following GOF Q-Q plot.

Output Screen for Gamma Distribution (Gamma-ROS Estimates)
Selected Options: Anderson Darling



Note: The font size of ND values in the above graph (and in all GOF graphs) is smaller than that of detected values.

8.5 Goodness-of-Fit Tests with DL/2 Estimates

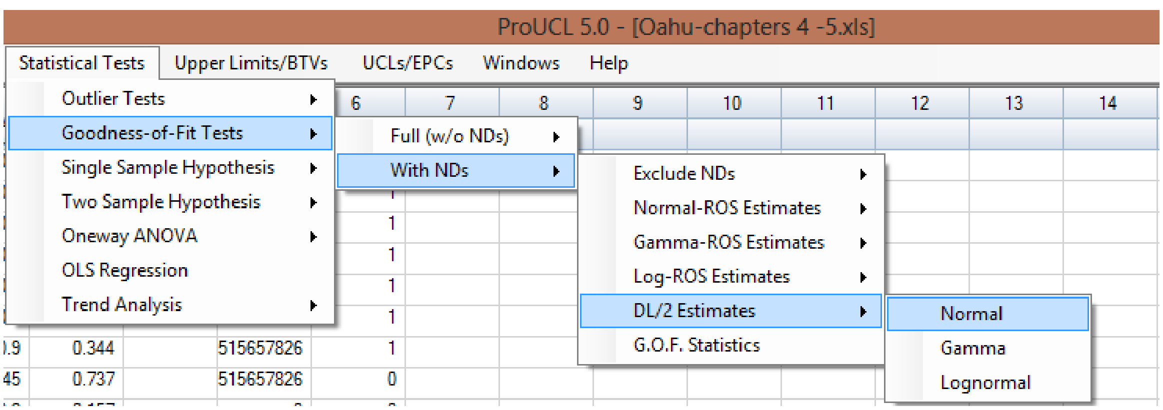
1. Click **Goodness-of-Fit Tests ► With NDs ► DL/2 Estimates**

2. Select the distribution to be tested: Normal, Gamma, or Lognormal

   - To test for normality, click on **Normal** from the drop-down menu list.
   - To test for lognormality, click on **Lognormal** from the drop-down menu list.
   - To test for a gamma distribution, click on **Gamma** from the drop-down menu list.

8.5.1 Normal or Lognormal Distribution (DL/2 Estimates)

1. Click **Goodness-of-Fit Tests ► With NDs ► DL/2 Estimates ► Normal or Lognormal**



2. The **Select Variables** screen (Chapter 3) will appear.

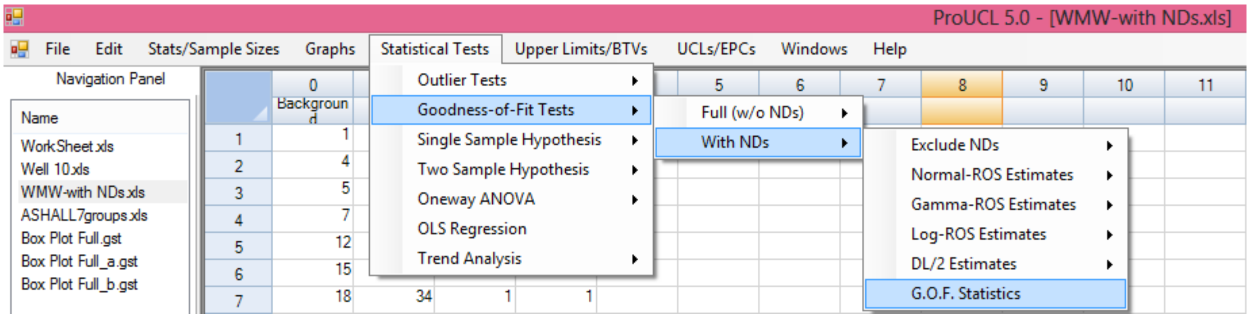
   - Select one or more variable(s) from the **Select Variables** screen.
   - If graphs have to be generated by using a group variable, then select a group variable by clicking the arrow below the **Select Group Column (Optional)** button. This will result in a drop-down list of available variables. The user should select and click on an appropriate variable representing a group variable.

   The rest of the process to determine the distribution (normal, lognormal, and gamma) of the data set thus obtained is the same as described in earlier sections.

8.6 Goodness-of-Fit Test Statistics

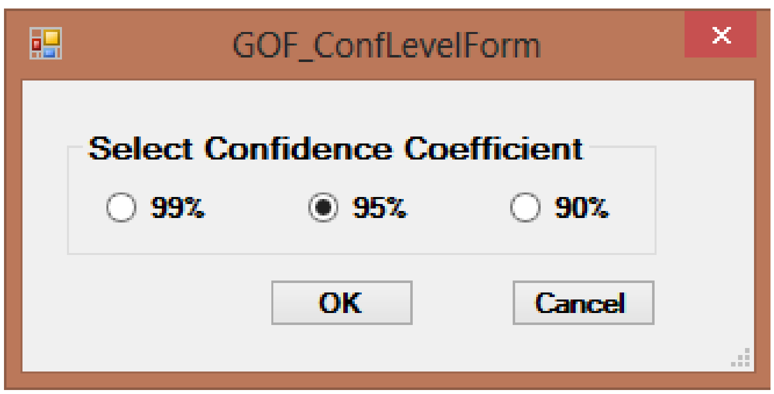
The **G.O.F.** option displays all GOF test statistics available in ProUCL. This option is used when the user does not know which GOF test to use to determine the data distribution. Based upon the information provided by the GOF test results, the user can perform an appropriate GOF test to generate GOF Q-Q plot based upon the hypothesized distribution. This option is available for uncensored as well as left censored data sets. Input and output screens associated with the G.O.F statistics option for data sets with NDs are summarized as follows.

1. Click **Goodness-of-Fit ► With NDs ► G.O.F. Statistics**



2. The **Select Variables** screen (Chapter 3) will appear.

   - Select one or more variable(s) from the **Select Variables** screen.
   - When the option button is clicked, the following window will be shown.



   - The default confidence level is **95%**.
   - Click the **OK** button to continue or the **Cancel** button to cancel the option.

Example 8-2e (continued). Consider the arsenic Oahu data set with NDs discussed earlier. Partial GOF test results, obtained using the **G.O.F. Statistics** option, are summarized in the following table.

Sample Output Screen for G.O.F. Test Statistics on Data Sets with Nondetect Observations

Arsenic

	Num Obs	Num Miss	Num Valid	Detects	NDs	% NDs
Raw Statistics	24	0	24	11	13	54.17%

	Number	Minimum	Maximum	Mean	Median	SD
Statistics (Non-Detects Only)	13	0.9	2	1.608	2	0.517
Statistics (Detects Only)	11	0.5	3.2	1.236	0.7	0.965
Statistics (All: NDs treated as DL value)	24	0.5	3.2	1.438	1.25	0.761
Statistics (All: NDs treated as DL/2 value)	24	0.45	3.2	1.002	0.95	0.699
Statistics (Normal ROS Imputed Data)	24	-0.0995	3.2	0.997	0.737	0.776
Statistics (Gamma ROS Imputed Data)	24	0.119	3.2	0.956	0.7	0.758
Statistics (Lognormal ROS Imputed Data)	24	0.349	3.2	0.972	0.7	0.718

	K hat	K Star	Theta hat	Log Mean	Log Stdv	Log CV
Statistics (Detects Only)	2.257	1.702	0.548	-0.0255	0.694	-27.26
Statistics (NDs = DL)	3.538	3.124	0.406	0.215	0.574	2.669
Statistics (NDs = DL/2)	3.233	2.857	0.31	-0.16	0.542	-3.381
Statistics (Gamma ROS Estimates)	2.071	1.84	0.461	--	--	--
Statistics (Lognormal ROS Estimates)	--	--	--	-0.209	0.571	-2.727

Normal GOF Test Results

	No NDs	NDs = DL	NDs = DL/2	Normal ROS
Correlation Coefficient R	0.887	0.948	0.833	0.928

	Test value	Crit. (0.05)	Conclusion with Alpha(0.05)
Shapiro-Wilk (Detects Only)	0.777	0.85	Data Not Normal
Shapiro-Wilk (NDs = DL)	0.89	0.916	Data Not Normal
Shapiro-Wilk (NDs = DL/2)	0.701	0.916	Data Not Normal
Shapiro-Wilk (Normal ROS Estimates)	0.868	0.916	Data Not Normal
Lilliefors (Detects Only)	0.273	0.251	Data Not Normal
Lilliefors (NDs = DL)	0.217	0.177	Data Not Normal
Lilliefors (NDs = DL/2)	0.335	0.177	Data Not Normal
Lilliefors (Normal ROS Estimates)	0.17	0.177	Data Appear Normal

Sample Output Screen for G.O.F. Test Statistics on Data Sets with Nondetect Observations (continued)

Gamma GOF Test Results				
	No NDs	NDs = DL	NDs = DL/2	Gamma ROS
Correlation Coefficient R	0.964	0.956	0.924	0.975
	Test value	Crit. (0.05)	Conclusion with Alpha(0.05)	
Anderson-Darling (Detects Only)	0.787	0.738		
Kolmogorov-Smirnov (Detects Only)	0.254	0.258	Detected Data appear Approximate Gamma Distı	
Anderson-Darling (NDs = DL)	0.98	0.75		
Kolmogorov-Smirnov (NDs = DL)	0.214	0.179	Data Not Gamma Distributed	
Anderson-Darling (NDs = DL/2)	1.492	0.751		
Kolmogorov-Smirnov (NDs = DL/2)	0.261	0.179	Data Not Gamma Distributed	
Anderson-Darling (Gamma ROS Estimates)	0.48	0.755		
Kolmogorov-Smirnov (Gamma ROS Est.)	0.126	0.18	Data Appear Gamma Distributed	

Lognormal GOF Test Results				
	No NDs	NDs = DL	NDs = DL/2	Log ROS
Correlation Coefficient R	0.939	0.959	0.933	0.963
	Test value	Crit. (0.05)	Conclusion with Alpha(0.05)	
Shapiro-Wilk (Detects Only)	0.86	0.85	Data Appear Lognormal	
Shapiro-Wilk (NDs = DL)	0.906	0.916	Data Not Lognormal	
Shapiro-Wilk (NDs = DL/2)	0.865	0.916	Data Not Lognormal	
Shapiro-Wilk (Lognormal ROS Estimates)	0.924	0.916	Data Appear Lognormal	
Lilliefors (Detects Only)	0.229	0.251	Data Appear Lognormal	
Lilliefors (NDs = DL)	0.214	0.177	Data Not Lognormal	
Lilliefors (NDs = DL/2)	0.217	0.177	Data Not Lognormal	
Lilliefors (Lognormal ROS Estimates)	0.143	0.177	Data Appear Lognormal	

Note: Substitution methods such as DL or DL/2 are not recommended.

Chapter 9

Single-Sample and Two-Sample Hypotheses Testing Approaches

This chapter illustrates single-sample and two-sample parametric and nonparametric hypotheses testing approaches as incorporated in the ProUCL software. All hypothesis tests are available under the **Statistical Tests** module of ProUCL 5.0/ProUCL 5.1. ProUCL software can perform these hypotheses tests on data sets with and without ND observations. It should be pointed out that, when one wants to use two-sample hypotheses tests on data sets with NDs, ProUCL assumes that samples from both of the samples/groups have ND observations. All this means is that, a ND column (with 0 or 1 entries only) needs to be provided for the variable in each of the two samples. This has to be done even if one of the samples (e.g., Site) has all detected entries; in this case the associated ND column will have all entries equal to '1.' This will allow the user to compare two groups (e.g., arsenic in background vs. site samples) with one of the groups having some NDs and the other group having all detected data.

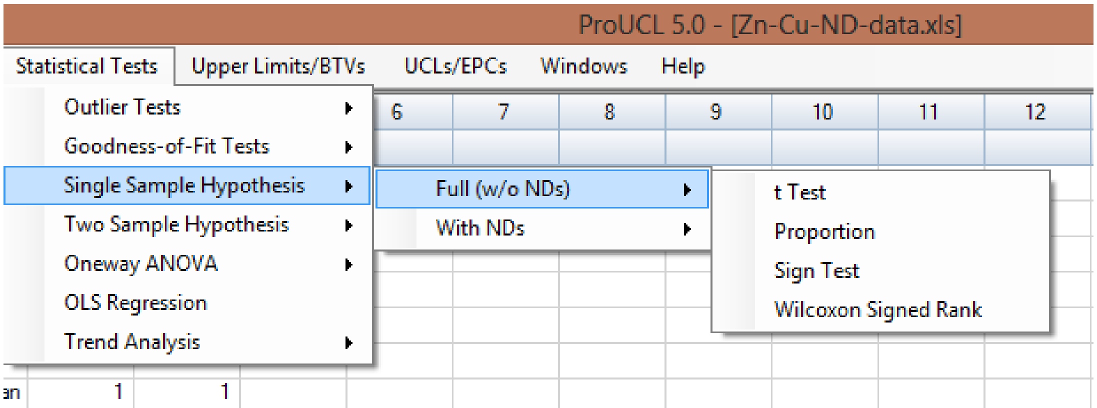
9.1 Single-Sample Hypotheses Tests

In many environmental applications, single-sample hypotheses tests are used to compare site data with pre-specified C_s or CLs. The single-sample hypotheses tests are useful when the environmental parameters such as the C_s, action level, or CLs are known, and the objective is to compare site concentrations with those known pre-established threshold values. Specifically, a t-test (or a sign test) may be used to verify the attainment of cleanup levels at an AOC after a remediation activity; and a test for proportion may be used to verify if the proportion of exceedances of an action level (or a compliance limit) by sample concentrations collected from an AOC (or a MW) exceeds a certain specified proportion (e.g., 1%, 5%, 10%).

ProUCL 5.1 can perform these hypotheses tests on data sets with and without ND observations. However, it should be noted that for single-sample hypotheses tests (e.g., sign test, proportion test) used to compare site mean/median concentration level with a C_s or a CL (e.g., proportion test), all NDs (if any) should lie below the cleanup standard, C_s. For proper use of these hypotheses testing approaches, the differences between these tests should be noted and understood. Specifically, a t-test or a Wilcoxon Signed Rank (WSR) test is used to compare the measures of location and central tendencies (e.g., mean, median) of a site area (e.g., AOC) to a cleanup standard, C_s, or action level also representing a measure of central tendency (e.g., mean, median); whereas, a proportion test compares if the proportion of site observations from an AOC exceeding a CL exceeds a specified proportion, P_0 (e.g., 5%, 10%). ProUCL has graphical methods that may be used to visually compare the concentrations of a site AOC with an action level. This can be done using a box plot of site data with horizontal lines displayed at action levels on the same graph. The details of the various single-sample hypotheses testing approaches are provided in the associated ProUCL Technical Guide.

9.1.1 Single-Sample Hypothesis Testing for Full Data without Nondetects

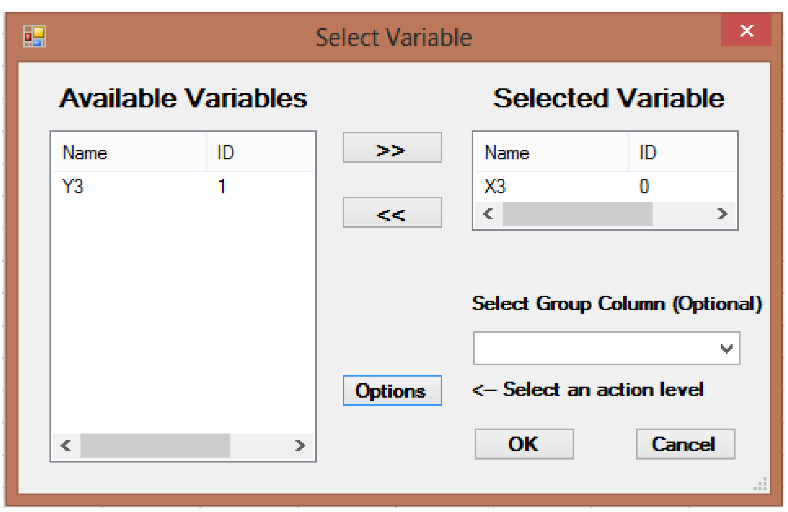
1. Click **Single Sample Hypothesis ► Full (w/o NDs)**



2. Select **Full (w/o NDs)** – This option is used for full data sets without nondetects.

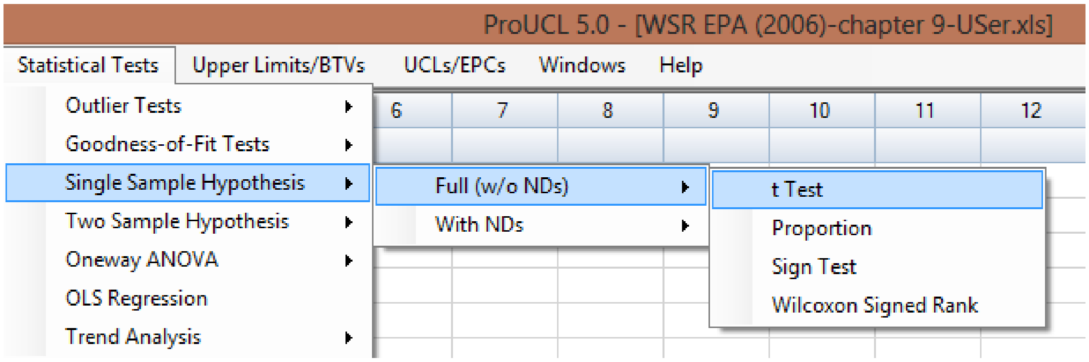
- To perform a t-test, click on **t-Test** from the drop-down menu as shown above.
- To perform a Proportion test, click on **Proportion** from the drop-down menu.
- To run a Sign test, click on **Sign test** from the drop-down menu.
- To run a Wilcoxon Signed Rank (WSR) test, click on **Wilcoxon Signed Rank** from the drop-down menu.

All single-sample hypothesis tests for uncensored and left-censored data sets can be performed by a group variable. The user selects a group variable by clicking the arrow below the **Select Group Column (Optional)** button. This will result in a drop-down list of available variables. The user should select and click on an appropriate variable representing a group variable.



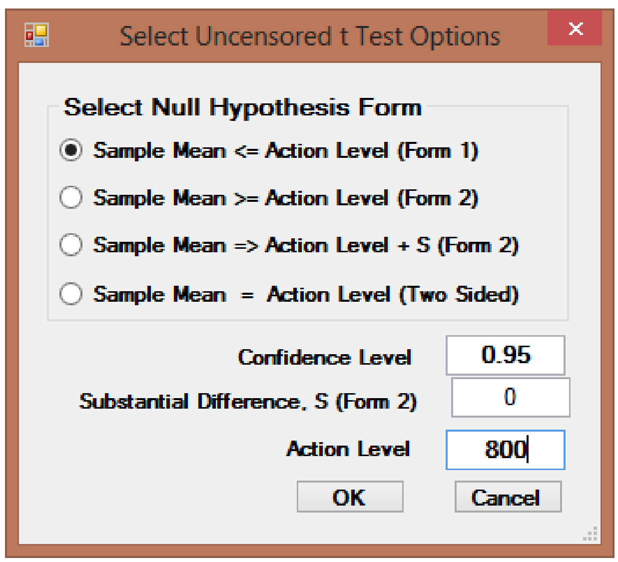
9.1.1.1 Single-Sample t-Test

1. Click **Single Sample Hypothesis ► Full (w/o NDs) ► t-Test**



2. The **Select Variables** screen will appear.

- Select variable(s) from the **Select Variables** screen.
- When the **Options** button is clicked, the following window will be shown.



  - Specify the **Confidence Level**; default is **0.95**.
  - Specify meaningful values for **Substantial Difference, S** and the **Action Level**. The default choice for S is "**0**."
  - Select form of Null Hypothesis; default is **Sample Mean <= Action Level (Form 1)**.
  - Click on **OK** button to continue or on **Cancel** button to cancel the test.

Example 9-1a. Consider the WSR data set described in EPA (2006a). One Sample t-test results are summarized as follows.

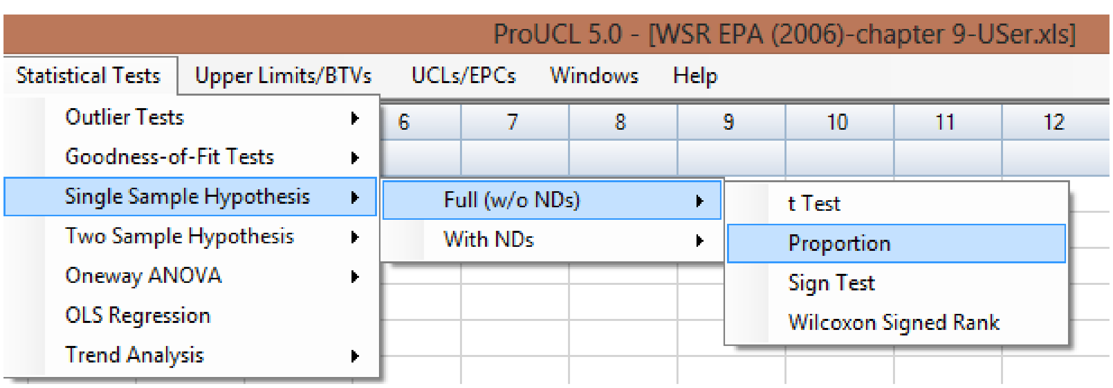
Output for Single-Sample t-Test (Full Data w/o NDs)

From File	WSR EPA (2006)-chapter 9-USer.xls
Full Precision	OFF
Confidence Coefficient	95%
Substantial Difference	0.000
Action Level	800.000
Selected Null Hypothesis	Mean <= Action Level (Form 1)
Alternative Hypothesis	Mean > the Action Level

WSR1	
One Sample t-Test	
Raw Statistics	
Number of Valid Observations	10
Number of Distinct Observations	10
Minimum	750
Maximum	1161
Mean	925.7
Median	888
SD	136.7
SE of Mean	43.24
H0: Sample Mean <= 800 (Form 1)	
Test Value	2.907
Degrees of Freedom	9
Critical Value (0.05)	1.833
P-Value	0.00869
Conclusion with Alpha = 0.05	
Reject H0, Conclude Mean > 800	
P-Value < Alpha (0.05)	

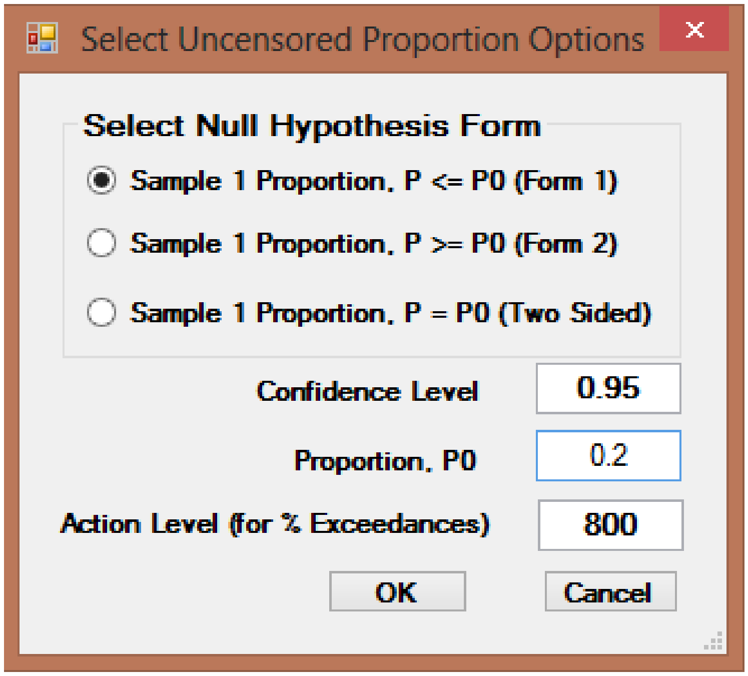
9.1.1.2 Single-Sample Proportion Test

1. Click **Single Sample Hypothesis ► Full (w/o NDs) ► Proportion**



2. The **Select Variables** screen will appear.

- Select variable(s) from the **Select Variables** screen.
- When the **Options** button is clicked, the following window will be shown.



- Specify the **Confidence level**; default is **0.95**.
- Specify the **Proportion** level and a meaningful **Action Level**.
- Select the form of Null Hypothesis; default is **Sample 1 Proportion <= P0 (Form 1)**.
- Click on **OK** button to continue or on **Cancel** button to cancel the test.

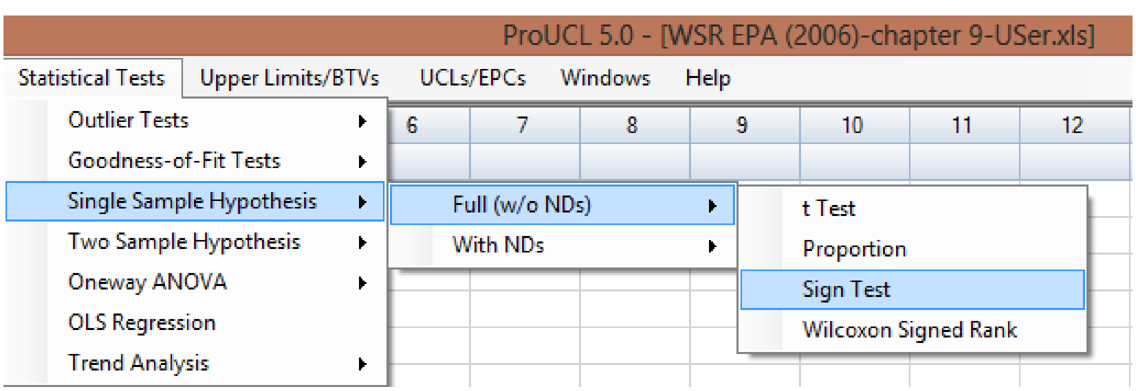
Example 9-1b (continued). Consider the WSR data set described in EPA (2006a). One Sample proportion test results are summarized as follows.

Output for Single-Sample Proportion Test (Full Data without NDs)

User Selected Options	
Date/Time of Computation	3/17/2013 10:29:38 PM
From File	WSR EPA (2006)-chapter 9-USer.xls
Full Precision	OFF
Confidence Coefficient	95%
User Specified Proportion	0.200 (P0 of Exceedances of Action Level)
Action/compliance Limit	800.000
Select Null Hypothesis	Sample Proportion, P of Exceedances of Action Level >= User Specified Proportion (Form 2)
Alternative Hypothesis	Sample Proportion, P of Exceedances of Action Level < the User Specified Proportion
WSR1	
One Sample Proportion Test	
Raw Statistics	
Number of Valid Observations	10
Number of Distinct Observations	10
Minimum	750
Maximum	1161
Mean	925.7
Median	888
SD	136.7
SE of Mean	43.24
Number of Exceedances	8
Sample Proportion of Exceedances	0.8
H0: Sample Proportion >= 0.2 (Form 2)	
P-Value Based Upon BD (Binomial Dist)	1
Conclusion with Alpha = 0.05	
Do Not Reject H0, Conclude Sample Proportion >= 0.2	
P-Value > Alpha (0.05)	

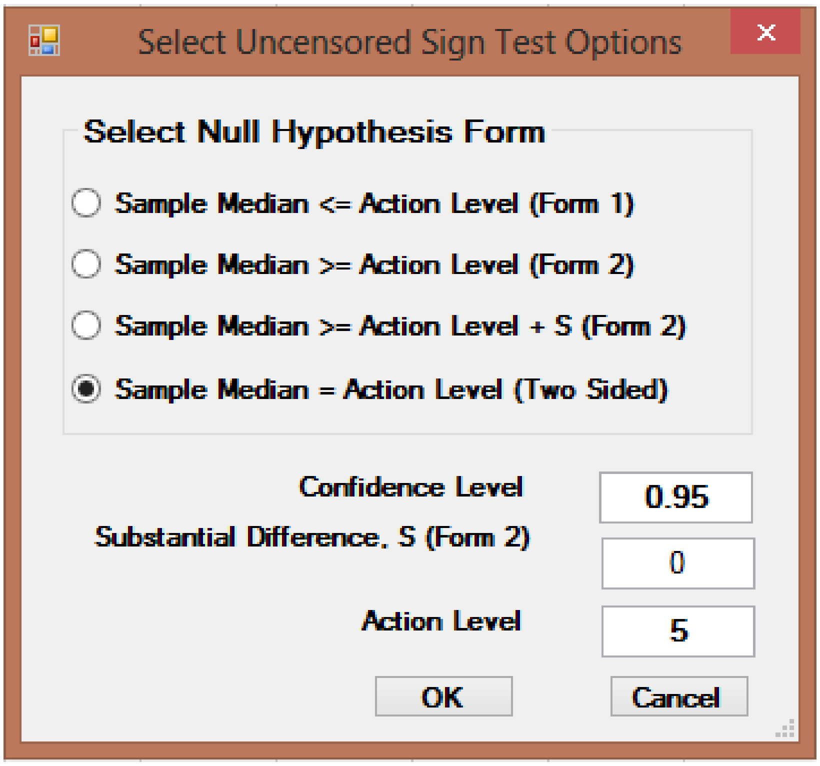
9.1.1.3 Single-Sample Sign Test

1. Click **Single Sample Hypothesis ► Full (w/o NDs) ► Sign test**



2. The **Select Variables** screen will appear.

- Select variable(s) from the **Select Variables** screen.
- When the **Options** button is clicked, the following window will be shown.



- Specify the **Confidence Level**; default choice is **0.95**.
- Specify meaningful values for **Substantial Difference, S** and **Action Level**.
- Select the form of Null Hypothesis; default is **Sample Median <= Action Level (Form 1)**.
- Click on **OK** button to continue or on **Cancel** button to cancel the test.

Example 9-1c (continued). Consider the WSR data set described in EPA (2006a). The Sign test results are summarized as follows.

Output for Single-Sample Sign Test (Full Data without NDs)

From File	WSR EPA (2006)-chapter 9-USer.xls
Full Precision	OFF
Confidence Coefficient	95%
Substantial Difference	0.000
Action Level	5.000
Selected Null Hypothesis	Median = Action/compliance Limit (2 Sided Alternative)
Alternative Hypothesis	Median <> Action/compliance Limit

WSR2

One Sample Sign Test

Raw Statistics

Number of Valid Observations	49
Number of Distinct Observations	44
Minimum	1.09
Maximum	7.5
Mean	5.048
Median	5.55
SD	1.775
SE of Mean	0.254
Number Above Action Level	29
Number Equal Action Level	0
Number Below Action Level	20

H0: Sample Median = 5

Large Sample Z Test Statistic	1.286
P-Value	0.199

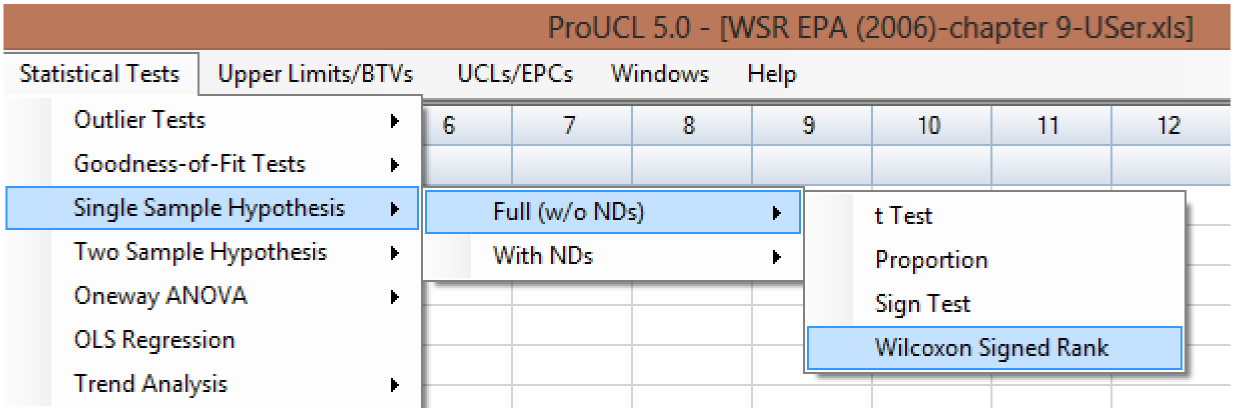
Conclusion with Alpha = 0.05

Do Not Reject H0 at the specified level of significance (0.05). Conclude Median = 5

P-Value > Alpha (0.05)

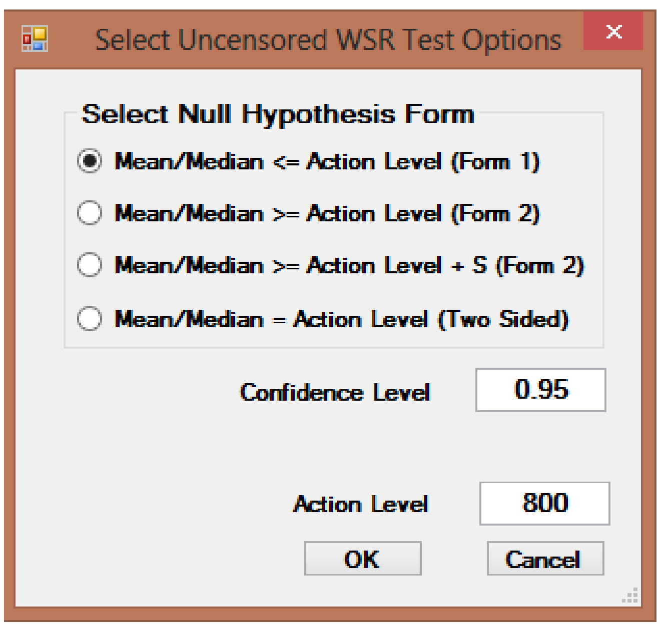
9.1.1.4 Single-Sample Wilcoxon Signed Rank (WSR) Test

1. Click **Single Sample Hypothesis ► Full (w/o NDs) ► Wilcoxon Signed Rank**



2. The **Select Variables** screen will appear.

- Select variable(s) from the **Select Variables** screen.
- When the **Options** button is clicked, the following window will be shown.



  - Specify the **Confidence Level**; default is **0.95**.
  - Specify meaningful values for **Substantial Difference, S,** and **Action Level**.
  - Select form of Null Hypothesis; default is **Mean/Median <= Action Level (Form 1)**.

o Click on **OK** button to continue or on **Cancel** button to cancel the test.

Example 9-1d (continued). Consider the WSR data set described in EPA (2006a). One Sample WSR test results are summarized as follows.

Output for Single-Sample Wilcoxon Signed Rank Test (Full Data without NDs)

Confidence Coefficient	95%
Substantial Difference	0.000
Action Level	800.000
Selected Null Hypothesis	Mean/Median <= Action Level (Form 1)
Alternative Hypothesis	Mean/Median > the Action Level

WSR1

One Sample Wilcoxon Signed Rank Test

Raw Statistics

Number of Valid Observations	10
Number of Distinct Observations	10
Minimum	750
Maximum	1161
Mean	925.7
Median	888
SD	136.7
SE of Mean	43.24
Number Above Action Level	8
Number Equal Action Level	0
Number Below Action Level	2
T-plus	50
T-minus	5

H0: Sample Mean/Median <= 800 (Form 1)

Exact Test Statistic	50
Critical Value (0.05)	45
P-Value	0.0098

Conclusion with Alpha = 0.05

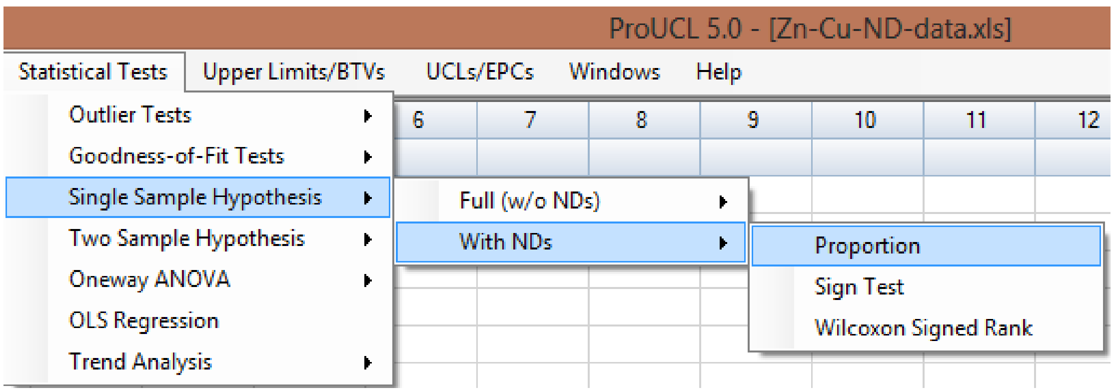
Reject H0, Conclude Mean/Median > 800

P-Value < Alpha (0.05)

9.1.2 Single-Sample Hypothesis Testing for Data Sets with Nondetects

Most of the one-sample tests such as the Proportion test and the Sign test on data sets with ND values assume that all ND observations lie below the specified action level, A_0. These single-sample tests are not performed if ND observations exceed the action levels. Single-sample hypothesis tests for data sets with NDs are shown in the following screen shot.

1. Click on **Single Sample Hypothesis ► With NDs**

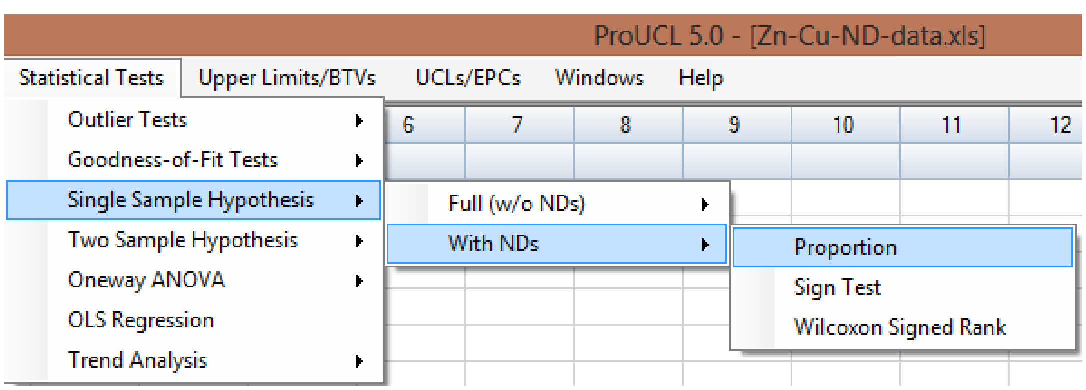


2. Select the With NDs option

- To perform a proportion test, click on **Proportion** from the drop-down menu.
- To perform a sign test, click on **Sign test** from the drop-down menu.
- To perform a Wilcoxon Signed Rank test, click on **Wilcoxon Signed Rank** from the drop-down menu list.

9.1.2.1 Single Proportion Test on Data Sets with NDs

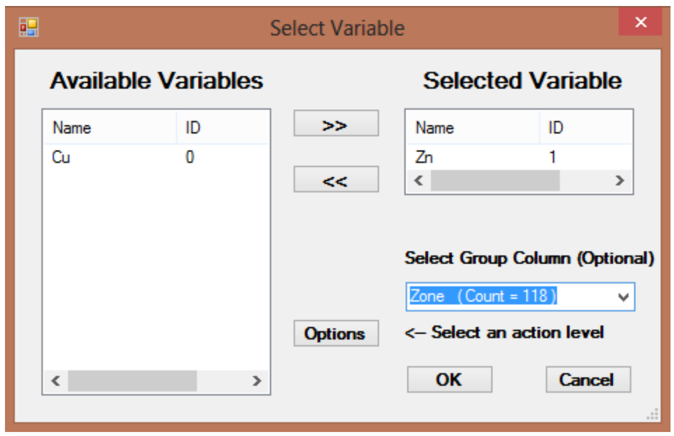
1. Click **Single Sample Hypothesis ► With NDs ► Proportion**



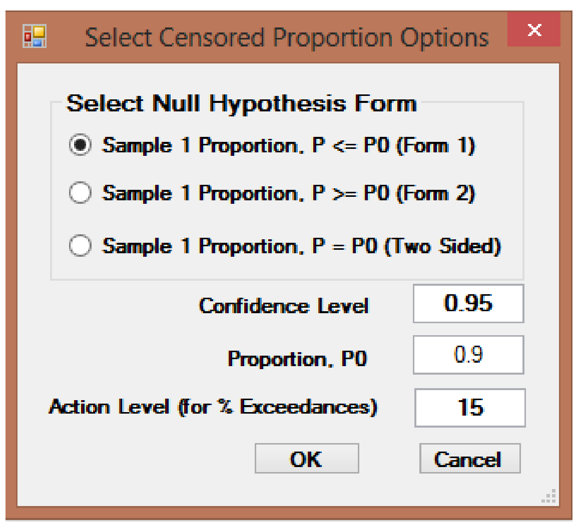
2. The **Select Variables** screen will appear.

- Select variable(s) from the **Select Variables** screen.

- If hypothesis test has to be performed by using a Group variable, then select a group variable by clicking the arrow below the **Select Group Column (Optional)** button. This will result in a drop-down list of available variables. The user should select and click on an appropriate variable representing a group variable. This option has been used in the following screen shot for the single-sample proportion test.



- When the **Options** button is clicked, the following window will be shown.



  - Specify the **Confidence Level**; default is **0.95**.

  - Specify meaningful values for **Proportion** and the **Action Level (=15 here).**

  - Select form of Null Hypothesis; default is **Sample 1 Proportion, P <= P0 (Form 1)**.

  - Click on **OK** button to continue or on **Cancel** button to cancel the test.

Example 9-2a. Consider the copper and zinc data set collected from two zones: Alluvial Fan and Basin Trough discussed in the literature (Helsel 2012, NADA in R [Helsel 2013]). This data set is used here to illustrate the one sample proportion test on a data set with NDs. The output sheet generated by ProUCL 5.1 is presented below.

Output for Single-Sample Proportion Test (with NDs) by Groups: Alluvial Fan and Basin Trough

User Selected Options	
Date/Time of Computation	3/18/2013 9:55:58 AM
From File	Zn-Cu-ND-data.xls
Full Precision	OFF
Confidence Coefficient	95%
User Specified Proportion	0.900 (P0 of Exceedances of Action Level)
Action Level	15.000
Select Null Hypothesis	Sample Proportion, P of Exceedances of Action Level <= User Specified Proportion (Form 1)
Alternative Hypothesis	Sample Proportion, P of Exceedances of Action Level > User Specified Proportion

Zn (alluvial fan)

One Sample Proportion Test

Note: All nondetects are treated as detects at values (e.g., DLs) included in Data File

Raw Statistics	
Number of Valid Data	67
Number of Missing Observations	1
Number of Distinct Data	19
Number of Non-Detects	16
Number of Detects	51
Percent Non-Detects	23.88%
Minimum Non-detect	3
Maximum Non-detect	10
Minimum Detect	5
Maximum Detect	620
Mean of Detects	27.88
Median of Detects	11
SD of Detects	85.02
Number of Exceedances	24
Sample Proportion of Exceedances	0.358

H0: Sample Proportion <= 0.9 (Form 1)

Large Sample z-Test Statistic	-14.58
Critical Value (0.05)	1.645
P-Value	1

Conclusion with Alpha = 0.05

Do Not Reject H0, Conclude Sample Proportion <= 0.9

P-Value > Alpha (0.05)

Zn (basin trough)

One Sample Proportion Test

Note: All nondetects are treated as detects at values (e.g., DLs) included in Data File

Raw Statistics	
Number of Valid Data	50
Number of Distinct Data	20
Number of Non-Detects	4
Number of Detects	46
Percent Non-Detects	8.00%
Minimum Non-detect	3
Maximum Non-detect	10
Minimum Detect	3
Maximum Detect	90
Mean of Detects	23.13
Median of Detects	20
SD of Detects	19.03
Number of Exceedances	27
Sample Proportion of Exceedances	0.54

H0: Sample Proportion <= 0.9 (Form 1)

Exact P-Value	1

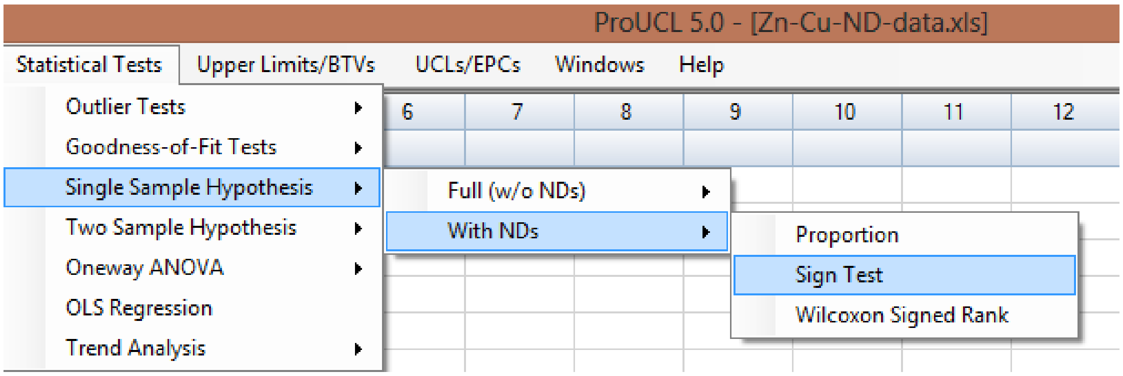
Conclusion with Alpha = 0.05

Do Not Reject H0, Conclude Sample Proportion <= 0.9

P-Value > Alpha (0.05)

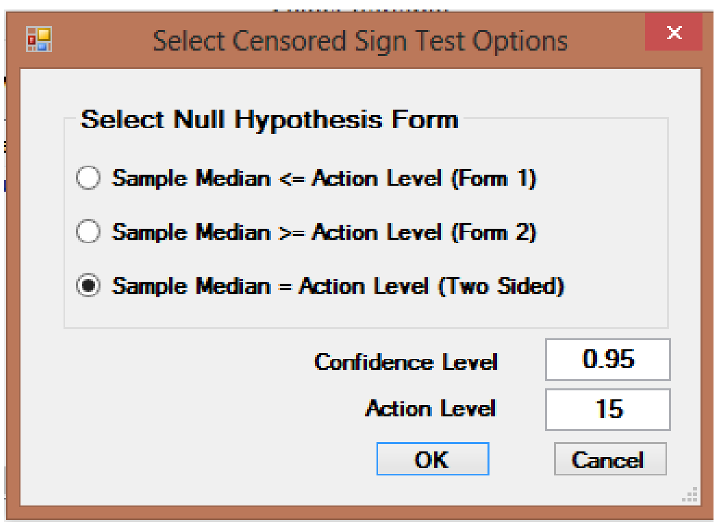
9.1.2.2 Single-Sample Sign Test with NDs

1. Click **Single Sample Hypothesis ► With NDs ► Sign test**



2. The **Select Variables** screen will appear.

- Select variable(s) from the **Select Variables** screen.
- When the **Options** button is clicked, the following window will be shown.



  - Specify the **Confidence Level**; default is **0.95**.
  - Select an **Action Level**.
  - Select the form of Null Hypothesis; default is **Sample Median <= Action Level (Form 1)**.
  - Click on **OK** button to continue or on **Cancel** button to cancel the test.

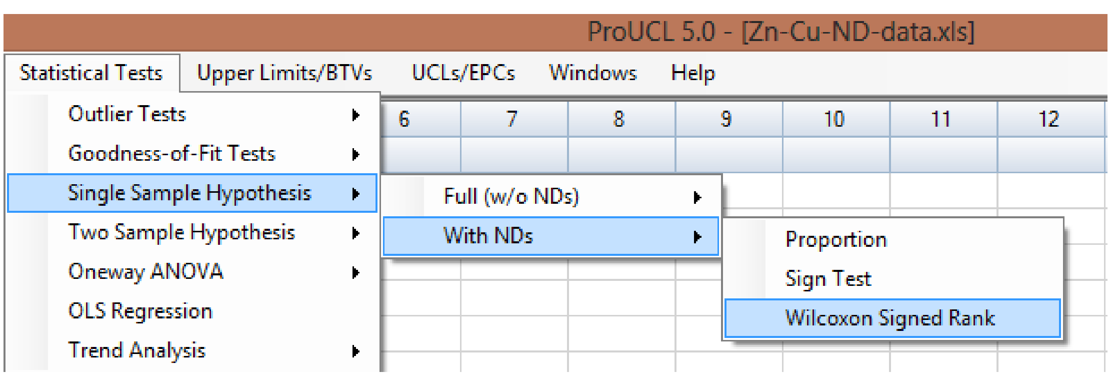
Example 9-2b (continued). Consider the copper and zinc data set collected from two zones: Alluvial Fan and Basin Trough discussed above. This data set is used here to illustrate the Single-Sample Sign test on a data set with NDs. The output sheet generated by ProUCL 5.0 follows.

Output for Single-Sample Sign Test (Data with Nondetects)

Selected Null Hypothesis	Median = Action/compliance Limit (Two Sided Alternative)
Alternative Hypothesis	Median <> Action/compliance Limit
Zn (alluvial fan)	
One Sample Sign Test	
Note: All nondetects are treated as detects at values (e.g., DLs) included in Data File	
Raw Statistics	
Number of Valid Data	67
Number of Missing Observations	1
Number of Distinct Data	19
Number of Non-Detects	16
Number of Detects	51
Percent Non-Detects	23.88%
Minimum Non-detect	3
Maximum Non-detect	10
Minimum Detect	5
Maximum Detect	620
Mean of Detects	27.88
Median of Detects	11
SD of Detects	85.02
Number Above Action Level	24
Number Equal Action Level	0
Number Below Action Level	43
H0: Sample Median = 15	
Standardized Test Value using Normal Appx.	-2.321
P-Value	0.0203
Conclusion with Alpha = 0.05	
Reject H0 at the specified level of significance (0.05). Conclude Median <> 15	
P-Value < Alpha (0.05)	

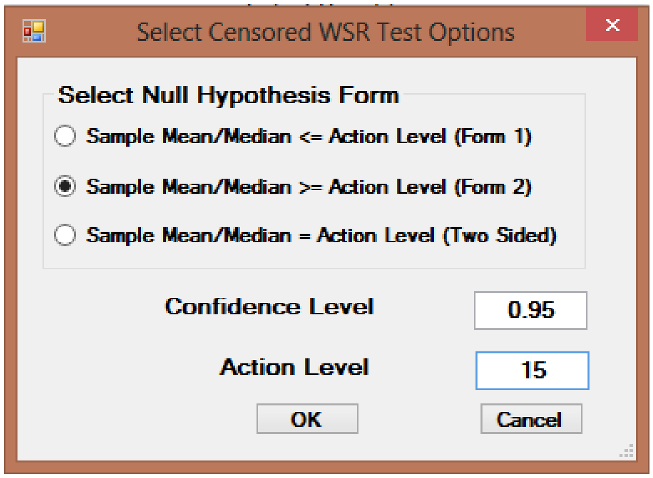
9.1.2.3 Single-Sample Wilcoxon Signed Rank Test with NDs

1. Click **Single Sample Hypothesis ► With NDs ► Wilcoxon Signed Rank**



2. The **Select Variables** screen will appear.

- Select variable(s) from the **Select Variables** screen.
- When the **Options** button is clicked, the following window will be shown.



  - Specify the **Confidence Level**; default is **0.95**.
  - Specify an **Action Level**.
  - Select form of Null Hypothesis; default is **Sample Mean/Median <= Action Level (Form 1)**.
  - Click on **OK** button to continue or on **Cancel** button to cancel the test.

Example 9-2c (continued). Consider the copper and zinc data set collected from two zones: Alluvial Fan and Basin Trough discussed earlier in this chapter. This data set is used here to illustrate one sample Wilcoxon Signed Rank test on a data set with NDs. The output sheet generated by ProUCL 5.0 is provided as follows.

Output for Single-Sample Wilcoxon Signed Rank Test (Data with Nondetects)

One Sample Wilcoxon Signed Rank Test for Data Sets with Non-Detects

User Selected Options	
Date/Time of Computation	3/18/2013 1:48:46 PM
From File	Zn-Cu-ND-data.xls
Full Precision	OFF
Confidence Coefficient	95%
Action Level	15.000
Selected Null Hypothesis	Mean/Median >= Action Level (Form 2)
Alternative Hypothesis	Mean/Median < the Action Level

Output for Single-Sample Wilcoxon Signed Rank Test (Data with Nondetects)- continued

Zn (basin trough)				
One Sample Wilcoxon Signed Rank Test				
Raw Statistics				
Number of Valid Data	50			
Number of Distinct Data	20			
Number of Non-Detects	4			
Number of Detects	46			
Percent Non-Detects	8.00%			
Minimum Non-detect	3			
Maximum Non-detect	10		H0: Sample Median >= 15 (Form 2)	
Minimum Detect	3			
Maximum Detect	90		Large Sample z-Test Statistic	1.269
Mean of Detects	23.13		Critical Value (0.05)	-1.645
Median of Detects	20		P-Value	0.898
SD of Detects	19.03			
Median of Processed Data used in WSR	18.5		Conclusion with Alpha = 0.05	
Number Above Action Level	27		Do Not Reject H0, Conclude Mean/Median >= 15	
Number Equal Action Level	1		P-Value > Alpha (0.05)	
Number Below Action Level	22			
T-plus	764		Dataset contains multiple Non-Detect values!	
T-minus	461		All NDs are replaced by their respective DL/2	

9.2 Two-Sample Hypotheses Testing Approaches

The two-sample hypotheses testing approaches available in ProUCL are described in this section. Like **Single-Sample Hypothesis**, the **Two-Sample Hypothesis** options are available under the **Statistical Tests** module of ProUCL 5.0/ProUCL 5.1. These approaches are used to compare the parameters and distributions of two populations (e.g., Background vs. AOC) based upon data sets collected from those populations. Several forms (Form 1 and Form 2, and Form 2 with Substantial Difference, S) of the two-sample hypothesis testing approaches are available in ProUCL. The methods are available for full-uncensored data sets as well as for data sets with ND observations with multiple detection limits.

- **Full (w/o NDs)** – performs parametric and nonparametric hypothesis tests on uncensored data sets consisting of all detected values. The following tests are available:
    - Student's t and Satterthwaite tests to compare the means of two populations (e.g. Background versus AOC).
    - F-test to the check the equality of dispersions of two populations.
    - Two-sample nonparametric Wilcoxon-Mann-Whitney (WMW) test. This test is equivalent to Wilcoxon Rank Sum (WRS) test.
- **With NDs** – performs hypothesis tests on left-censored data sets consisting of detected and ND values. The following tests are available:
    - Wilcoxon-Mann-Whitney test. All observations (including detected values) below the highest detection limit are treated as ND (less than the highest DL) values.

- o Gehan’s test is useful when multiple detection limits may be present.

- o Tarone-Ware test is useful when multiple detection limits may be present.

The details of these methods can be found in the ProUCL Technical Guides (2013, 2015) and are also available in EPA (2002b, 2006a, 2009a, 2009b). It is emphasized that the use of informal graphical displays (e.g., side-by-side box plots, multiple Q-Q plots) should always accompany the formal hypothesis testing approaches listed above. This is especially warranted when data sets may consist of NDs with multiple detection limits and observations from multiple populations (e.g., mixture samples collected from various onsite locations) and outliers.

Notes: As mentioned before, when one wants to use two-sample hypotheses tests on data sets with NDs, ProUCL assumes that samples from both of the groups have ND observations. This may not be the case, as data from a polluted site may not have any ND observations. ProUCL can handle such data sets; the user will have to provide a ND column (with 0 or 1 entries only) for the selected variable of each of the two samples/groups. Thus when one of the samples (e.g., site arsenic) has no ND value, the user supplies an associated ND column with all entries equal to '1'. This will allow the user to compare two groups (e.g., arsenic in background vs. site samples) with one of the groups having some NDs and the other group having all detected data.

9.2.1 Two-Sample Hypothesis Tests for Full Data

Full (w/o NDs): This option is used to analyze data sets consisting of all detected values. The following two-sample tests are available in ProUCL 5.1.

- Student’s t and Satterthwaite tests to compare the means of two populations (e.g., Background versus AOC).

- F-test is also available to test the equality of dispersions of two populations.

- Two-sample nonparametric Wilcoxon-Mann-Whitney (WMW) test.

- **Student’s t-Test**

  - o Based upon collected data sets, this test is used to compare the mean concentrations of two populations/groups provided the populations are normally distributed. The data sets are represented by independent random observations, X1, X2, . . . , Xn collected from one population (e.g., site), and independent random observations, Y1, Y2, . . . , Ym collected from another (e.g., background) population. The same terminology is used for all other two-sample tests discussed in the following sub-sections of this section.

  - o Student’s t-test also assumes that the spreads (variances) of the two populations are approximately equal.

  - o The F-test can be used to the check the equality of dispersions of two populations. A couple of other tests (e.g., Levene 1960) are also available in the literature to compare the variances of two populations. Since the F-test performs fairly well, other tests are not included in the ProUCL software. For more details refer to ProUCL Technical Guides.

- **Satterthwaite t-Test**

  This test is used to compare the means of two populations when the variances of those populations may not be equal. As mentioned before, the F-distribution based test can be used to verify the equality of dispersions of the two populations. However, this test alone is more powerful test to compare the means of two populations.

- **Test for Equality of two Dispersions (F-test)**

  - This test is used to determine whether the true underlying variances of two populations are equal. Usually the F-test is employed as a preliminary test, before conducting the two-sample t-test for testing the equality of means of two populations.

  - The assumptions underlying the F-test are that the two-samples represent independent random samples from two normal populations. The F-test for equality of variances is sensitive to departures from normality.

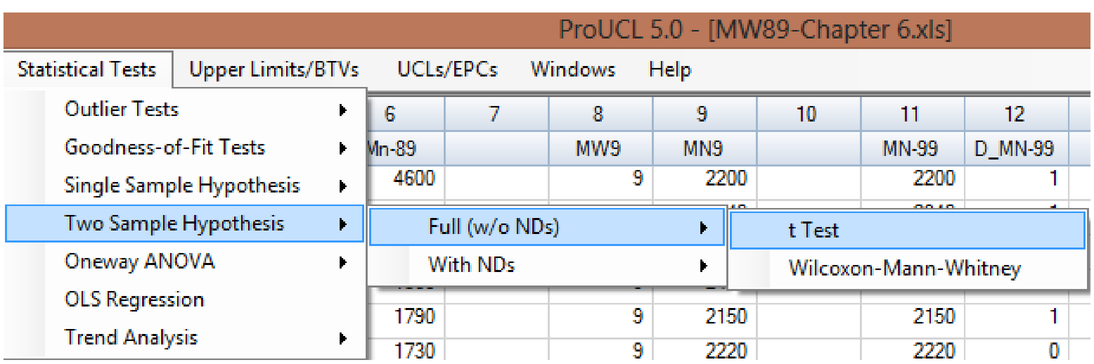
- **Two-Sample Nonparametric WMW Test**

  - This test is used to determine the comparability of the two continuous data distributions. This test also assumes that the shapes (e.g., as determined by spread, skewness, and graphical displays) of the two populations are roughly equal. The test is often used to determine if the measures of central locations (mean, median) of the two populations are significantly different.

  - The Wilcoxon-Mann-Whitney test does not assume that the data are normally or log-normally distributed. For large samples (e.g., ≥ 20), the distribution of the WMW test statistic can be approximated by a normal distribution.

Notes: The use of the tests listed above is not recommended on log-transformed data sets, especially when the parameters of interests are the population means. In practice, cleanup and remediation decisions have to be made in the original scale based upon statistics and estimates computed in the original scale. The equality of means in log-scale does not necessarily imply the equality of means in the original scale.

1. Click on **Two Sample Hypothesis ► Full (w/o NDs)**



2. Select the **Full (w/o NDs)** option

- To perform a t-test, click on **t Test** from the drop-down menu.

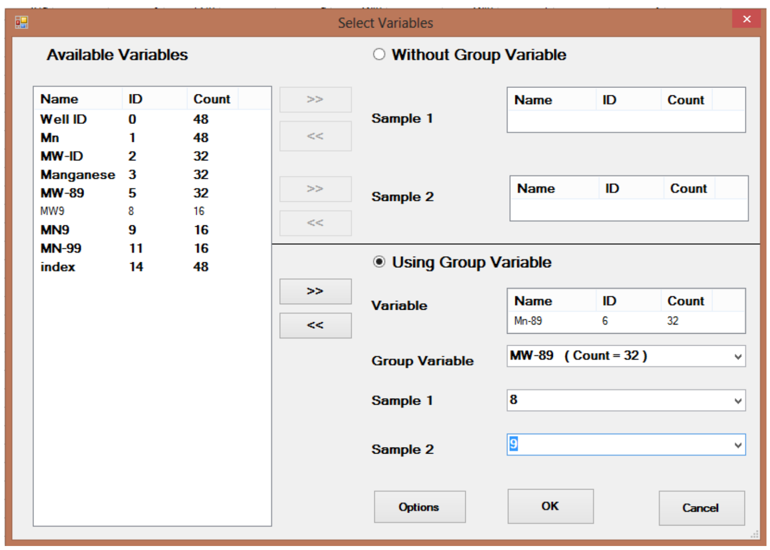
- To perform a Wilcoxon-Mann-Whitney, click on **Wilcoxon-Mann-Whitney** from the drop-down menu list.

9.2.1.1 *Two-Sample t-Test without NDs*

1. Click on **Two Sample Hypothesis ► Full (w/o NDs) ► t Test**

2. The **Select Variables** screen will appear.

- Select variable(s) from the **Select Variables** screen.



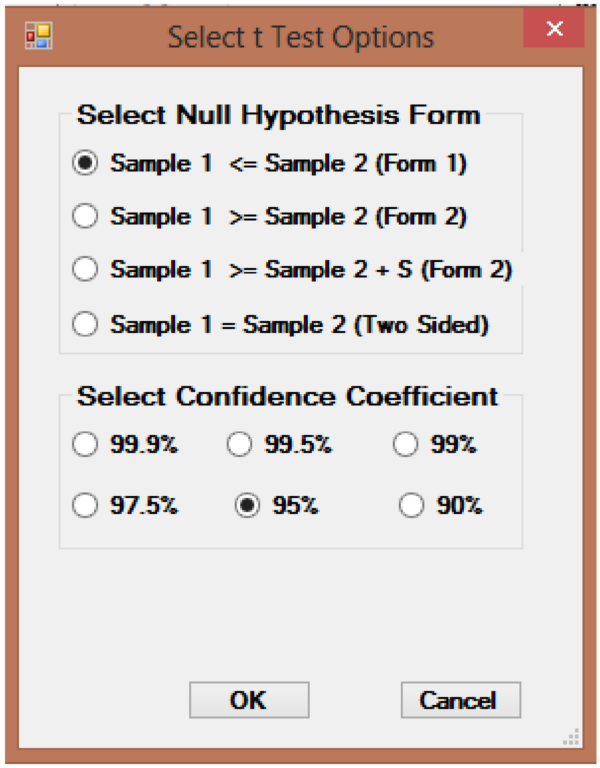
- **Without Group Variable**: This option is used when the sampled data of the variable (e.g., lead) for the two populations (e.g., site vs. background) are given in separate columns.

- **With Group Variable**: This option is used when sampled data of the variable (e.g., lead) for the two populations (e.g., site vs. background) are given in the same column.

- The values are separated into different populations (groups) by the values of an associated Group ID Variable. The group variable may represent several populations (e.g., background, surface, subsurface, silt, clay, sand, several AOCs, MWs). The user can compare two groups at a time by using this option.

- When the **Group** option is used, the user then selects a variable by using the **Group Variable Option**. The user should select an appropriate variable representing a group variable. The user can use letters, numbers, or alphanumeric labels for the group names.

- When the **Options** button is clicked, the following window will be shown.



- Specify a useful **Substantial Difference, S** value. The default choice is **0**.

- Select the **Confidence Coefficient**. The default choice is **95%**.

- Select the form of Null Hypothesis. The default is **Sample 1 <= Sample 2 (Form 1)**.

- Click on **OK** button to continue or on **Cancel** button to cancel the option.

- Click on **OK** button to continue or on **Cancel** button to cancel the Sample 1 versus Sample 2 Comparison.

Example 9-3. Consider the manganese concentrations data set collected from three wells: MW1, an upgradient well, and MW8 and MW9, two downgradient wells. The two-sample t-test results, comparing Mn concentrations in MW8 vs. MW9, are described as follows.

Output for Two-Sample t-Test (Full Data without NDs)

Confidence Coefficient	95%
Substantial Difference (S)	0.000
Selected Null Hypothesis	Sample 1 Mean = Sample 2 Mean (Two Sided Alternative)
Alternative Hypothesis	Sample 1 Mean <> Sample 2 Mean

Sample 1 Data: Mn-89(8)

Sample 2 Data: Mn-89(9)

Raw Statistics

	Sample 1	Sample 2
Number of Valid Observations	16	16
Number of Distinct Observations	16	15
Minimum	1270	1050
Maximum	4600	3080
Mean	1998	1968
Median	1750	2055
SD	838.8	500.2
SE of Mean	209.7	125

Sample 1 vs Sample 2 Two-Sample t-Test

H0: Mean of Sample 1 = Mean of Sample 2

		t-Test	Lower C.Val	Upper C.Val	
Method	DF	Value	t (0.025)	t (0.975)	P-Value
Pooled (Equal Variance)	30	0.123	-2.042	2.042	0.903
Welch-Satterthwaite (Unequal Varian	24.5	0.123	-2.064	2.064	0.903

Pooled SD: 690.548

Conclusion with Alpha = 0.050

Student t (Pooled): Do Not Reject H0, Conclude Sample 1 = Sample 2

Welch-Satterthwaite: Do Not Reject H0, Conclude Sample 1 = Sample 2

Test of Equality of Variances

Variance of Sample 1	703523
Variance of Sample 2	250190

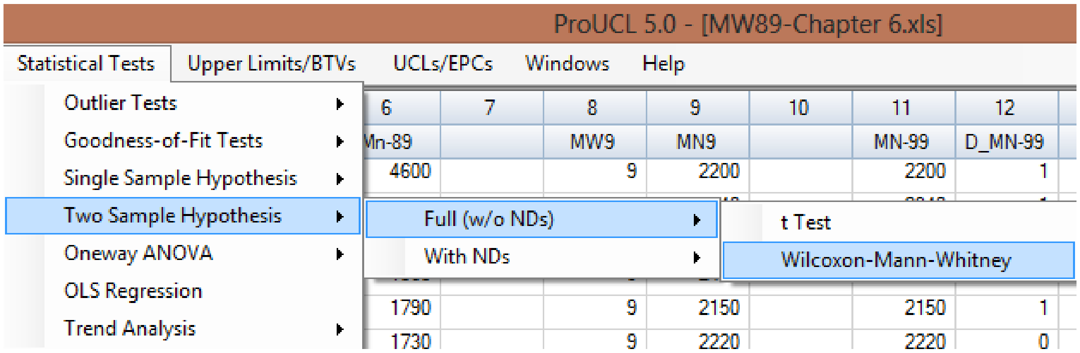
Numerator DF	Denominator DF	F-Test Value	P-Value
15	15	2.812	0.054

Conclusion with Alpha = 0.05

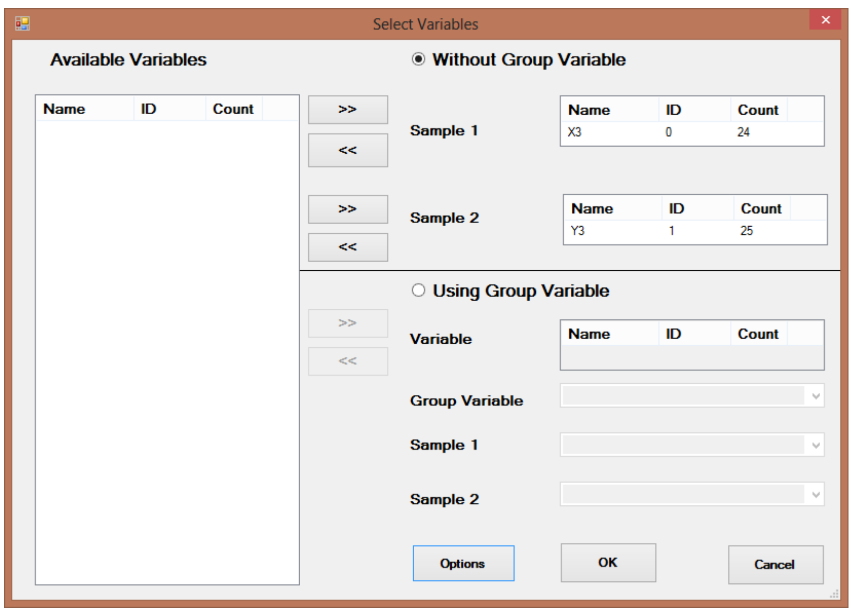
Two variances appear to be equal

9.2.1.2 Two-Sample Wilcoxon-Mann-Whitney (WMW) Test without NDs

1. Click on **Two Sample Hypothesis Testing ► Full (w/o NDs) ► Wilcoxon-Mann-Whitney**



2. The **Select Variables** screen will appear.

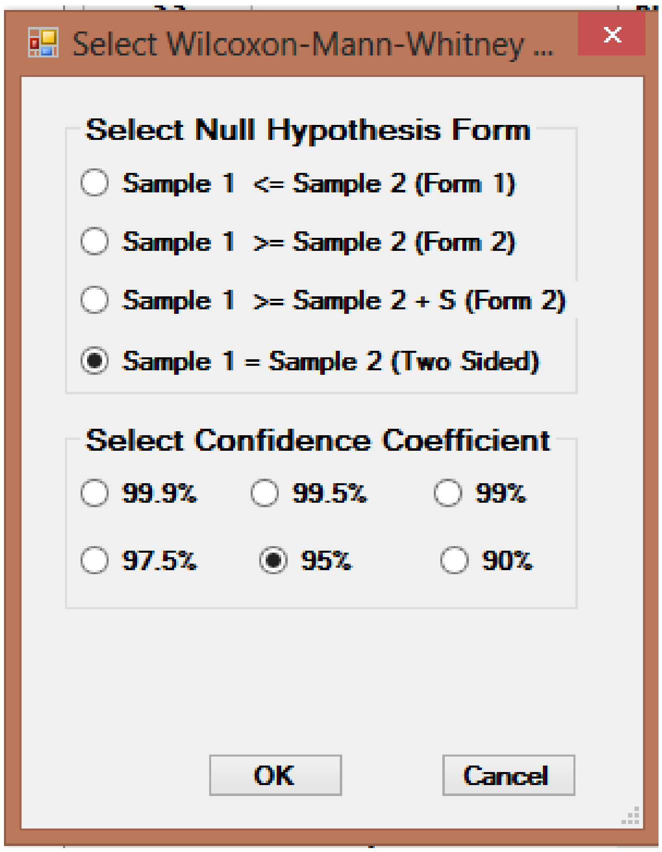


- Select variable(s) from the Select Variables screen.
- **Without Group Variable**: This option is used when the data values of the variable (arsenic) are given in separate columns.
- **With Group Variable**: This option is used when data of the variable (arsenic) are given in the same column. The values are separated into different samples (groups) by the values of an associated Group Variable.
- When the Group option is used, the user then selects a group variable/ID by using the **Group Variable Option**. The user should select an appropriate variable representing a

group variable. The user can use letters, numbers, or alphanumeric labels for the group names.

Notes: ProUCL documents have been written using environmental terminology such as performing background versus site comparisons. However, all tests and procedures incorporated in ProUCL can be used on data sets from any other application. For other applications such as comparing a new treatment drug versus older treatment drug, the group variable may represent the two groups: Control Drug and New Drug.

- When the Options button is clicked, the following window is shown.



  - Specify a **Substantial Difference, S** value. The default choice is **0**.
  - Choose the **Confidence Coefficient**. The default choice is **95%**.
  - Select the form of Null Hypothesis. The default is **Sample 1<= Sample 2 (Form 1)**.
  - Click on **OK** button to continue or on **Cancel** button to cancel the selected options.
- Click on **OK** to continue or on **Cancel** to cancel Sample 1 vs. Sample 2 comparison.

Example 9- 4. The two-sample Wilcoxon Mann Whitney (WMW) test results on a data set with ties are summarized as follows.

Output for Two-Sample Wilcoxon-Mann-Whitney Test (Full Data with ties)

Substantial Difference	0.000
Selected Null Hypothesis	Sample 1 Mean/Median = Sample 2 Mean/Median (Two Sided Alternative)
Alternative Hypothesis	Sample 1 Mean/Median <> Sample 2 Mean/Median

Sample 1 Data: X3
Sample 2 Data: Y3

Raw Statistics

	Sample 1	Sample 2
Number of Valid Observations	24	25
Number of Distinct Observations	18	19
Minimum	5.687	1.85
Maximum	31.2	79.06
Mean	17.38	39.8
Median	17.56	44.63
SD	7.421	19.39
SE of Mean	1.515	3.878

Wilcoxon-Mann-Whitney (WMW) Test

H0: Mean/Median of Sample 1 = Mean/Median of Sample 2

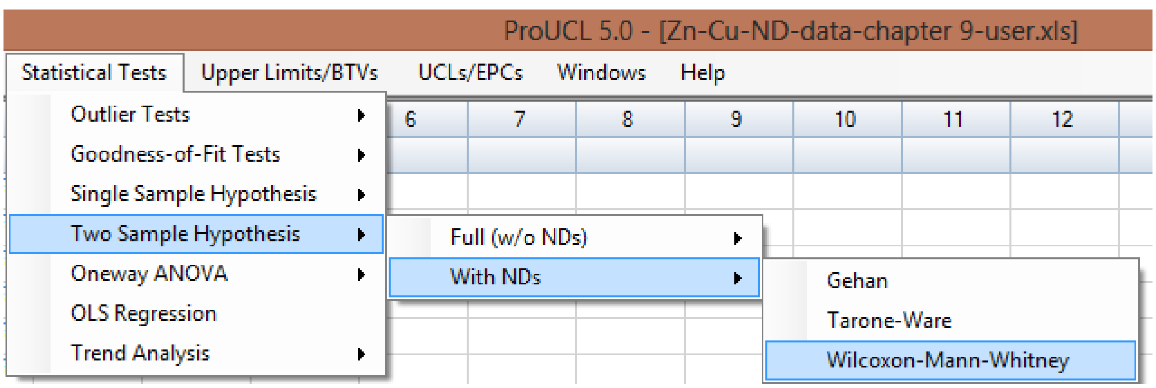
Sample 1 Rank Sum W-Stat	396
WMW U-Stat	96
Standardized WMW U-Stat	-4.083
Mean (U)	300
SD(U) - Adj ties	49.97
Lower Approximate U-Stat Critical Value (0.025)	-1.96
Upper Approximate U-Stat Critical Value (0.975)	1.96
P-Value (Adjusted for Ties)	4.4474E-5

Conclusion with Alpha = 0.05
Reject H0, Conclude Sample 1 <> Sample 2

P-Value < alpha (0.05)

9.2.2 *Two-Sample Hypothesis Testing for Data Sets with Nondetects*

1. Click **Two Sample Hypothesis ► With NDs**

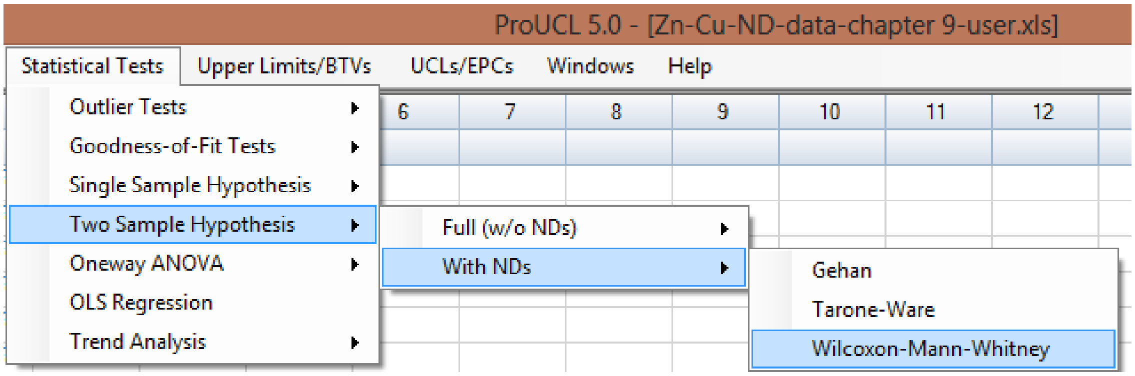


2. Select the **With NDs** option. A list of available tests will appear (shown above).

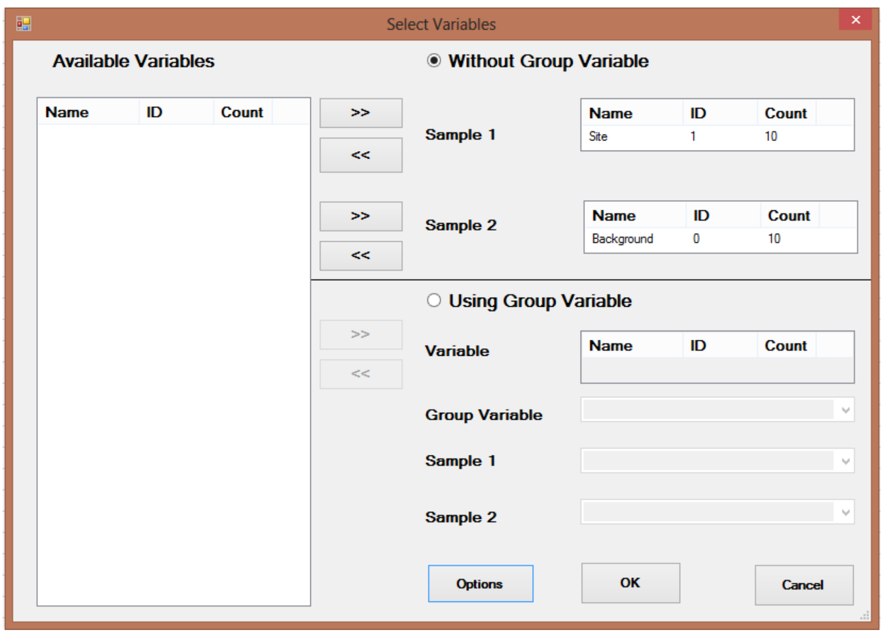
   - To perform a Wilcoxon-Mann-Whitney test, click on **Wilcoxon-Mann-Whitney** from the drop-down menu list.
   - To perform a Gehan test, click on **Gehan** from the drop-down menu.
   - To perform a Tarone-Ware test, click on **Tarone-Ware** from the drop-down menu.

9.2.2.1 Two-Sample Wilcoxon-Mann-Whitney Test with Nondetects

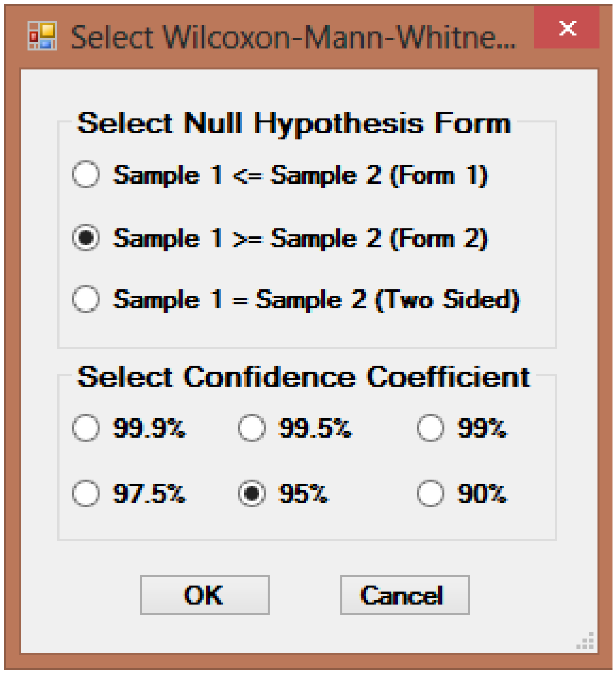
1. Click **Two Sample Hypothesis ► With NDs ► Wilcoxon-Mann-Whitney**



2. The **Select Variables** screen shown below will appear.



- Select variable(s) from the **Select Variables** screen.
- **Without Group Variable**: This option is used when the data values of the variable (e.g., TCDD 2,3,7,8) for the site and the background are given in separate columns.
- **With Group Variable**: This option is used when data values of the variable (TCDD 2, 3, 7, 8) are given in the same column. The values are separated into different samples (groups) by the values of an associated **Group Variable**. When using this option, the user should select an appropriate variable representing groups such as AOC1, AOC2, AOC3 etc.
- When the **Options** button is clicked, the following window will be shown.



  - Choose the **Confidence Coefficient**. The default choice is **95%**.
  - Select the form of Null Hypothesis. The default is **Sample 1 <= Sample 2 (Form 1)**.
  - Click on **OK** button to continue or on **Cancel** button to cancel the selected options.
- Click on **OK** to continue or on **Cancel** to cancel the Sample 1 vs. Sample 2 comparison.

Example 9-5. Consider a two sample data set with nondetects and multiple detection limits. Since the data sets have more than one detection limit, the WMW test is not recommended for this data set. However, sometimes, the users tend to use the WMW test on data sets with multiple detection limits. The WMW test results are summarized as follows.

Output for Two-Sample Wilcoxon-Mann-Whitney Test (with Nondetects)

Date/Time of Computation	3/18/2013 6:43:04 PM
From File	WMW-NDs-Chapter 9-user_a.xls
Full Precision	OFF
Confidence Coefficient	95%
Selected Null Hypothesis	Sample 1 Mean/Median >= Sample 2 Mean/Median (Form 2)
Alternative Hypothesis	Sample 1 Mean/Median < Sample 2 Mean/Median

Sample 1 Data: Site
Sample 2 Data: Background

Raw Statistics

	Sample 1	Sample 2
Number of Valid Data	11	11
Number of Non-Detects	3	3
Number of Detect Data	8	8
Minimum Non-Detect	4	4
Maximum Non-Detect	11	9
Percent Non-detects	27.27%	27.27%
Minimum Detect	2	1
Maximum Detect	43	27
Mean of Detects	27	15.5
Median of Detects	29.5	16.5
SD of Detects	13.71	9.196

WMW test is meant for a Single Detection Limit Case
of Gehan or T-W test is suggested when multiple detection limits are pres
All observations <= 11 (Max DL) are ranked the same

WMW test is meant for a Single Detection Limit Case
Use of Gehan or T-W test is suggested when multiple detection limits are present
All observations <= 11 (Max DL) are ranked the same

Wilcoxon-Mann-Whitney (WMW) Test

H0: Mean/Median of Sample 1 >= Mean/Median of Sample 2

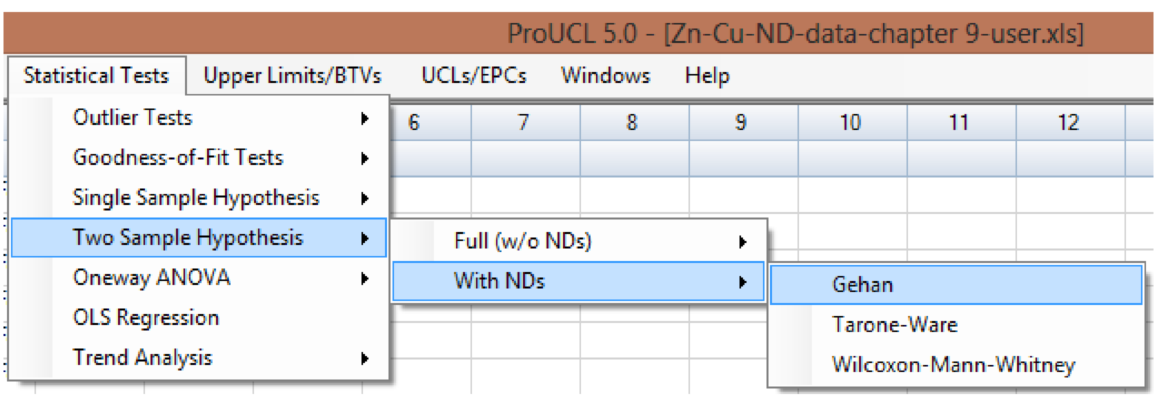
Sample 1 Rank Sum W-Stat	144.5
WMW U-Stat	78.5
Mean (U)	60.5
SD(U) - Adj ties	15.22
WMW U-Stat Critical Value (0.05)	35
Standardized WMW U-Stat	1.191
Approximate P-Value	0.883

Conclusion with Alpha = 0.05
Do Not Reject H0, Conclude Sample 1 >= Sample 2

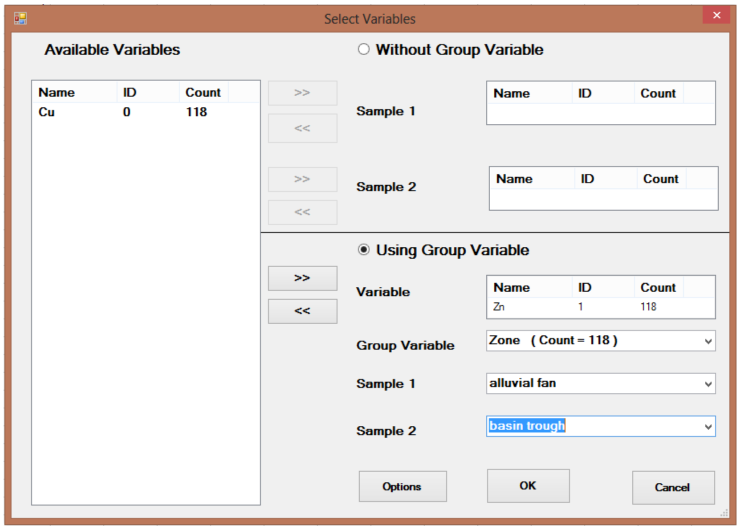
Notes**:** In the WMW test, all observations below the largest detection limit are considered as NDs (potentially including some detected values) and hence they all receive the same average rank. This action tends to reduce the associated power of the WMW test considerably. This in turn may lead to an incorrect conclusion.

9.2.2.2 Two-Sample Gehan Test for Data Sets with Nondetects

1. Click **Two Sample Hypothesis ► With NDs ► Gehan**



2. The **Select Variables** screen will appear.

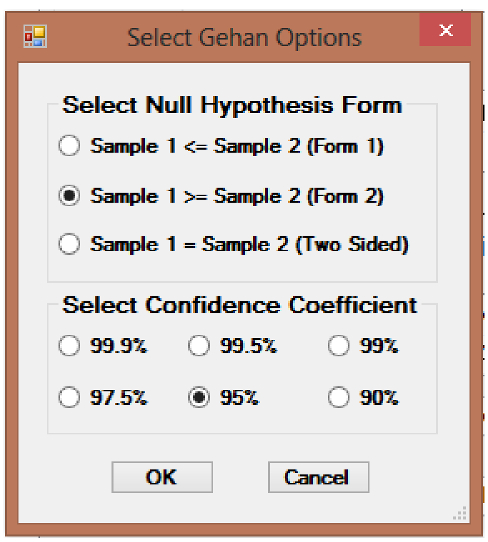


- Select variable(s) from the **Select Variables** screen.

- **Without Group Variable**: This option is used when the data values of the variable (Zinc) for the two data sets are given in separate columns.

- **With Group Variable**: This option is used when data values of the variable (Zinc) for the two data sets are given in the same column. The values are separated into different samples (groups) by the values of an associated **Group Variable**. When using this option, the user should select a group variable representing groups/populations such as Zone 1, Zone2, Zone3, etc.

- When the **Options** button is clicked, the following window will be shown.



- Choose the **Confidence Coefficient**. The default choice is **95%**.
- Select the form of Null Hypothesis. The default is **Sample 1 <= Sample 2 (Form 1)**.
- Click on **OK** button to continue or on **Cancel** button to cancel selected options.

- Click on the **OK** button to continue or on the **Cancel** button to cancel the Sample 1 vs. Sample 2 Comparison.

Example 9-6a. Consider the copper and zinc data set collected from two zones: Alluvial Fan and Basin Trough discussed in the literature (Helsel 2012). This data set is used here to illustrate the Gehan two-sample test. The output sheet generated by ProUCL 5.0 (similar sheet is generated using ProUCL 5.1, therefore the following output is not replaced) follows.

Output for Two-Sample Gehan Test (with Nondetects)

Confidence Coefficient	95%	
Selected Null Hypothesis	Sample 1 Mean/Median >= Sample 2 Mean/Median (Form 2)	
Alternative Hypothesis	Sample 1 Mean/Median < Sample 2 Mean/Median	

Sample 1 Data: Zn(alluvial fan)
Sample 2 Data: Zn(basin trough)

Raw Statistics

	Sample 1	Sample 2
Number of Valid Data	67	50
Number of Missing Observations	1	0
Number of Non-Detects	16	4
Number of Detect Data	51	46
Minimum Non-Detect	3	3
Maximum Non-Detect	10	10
Percent Non-detects	23.88%	8.00%
Minimum Detect	5	3
Maximum Detect	620	90
Mean of Detects	27.88	23.13
Median of Detects	11	20
SD of Detects	85.02	19.03

Sample 1 vs Sample 2 Gehan Test

H0: Mean of Sample 1 >= Mean of background

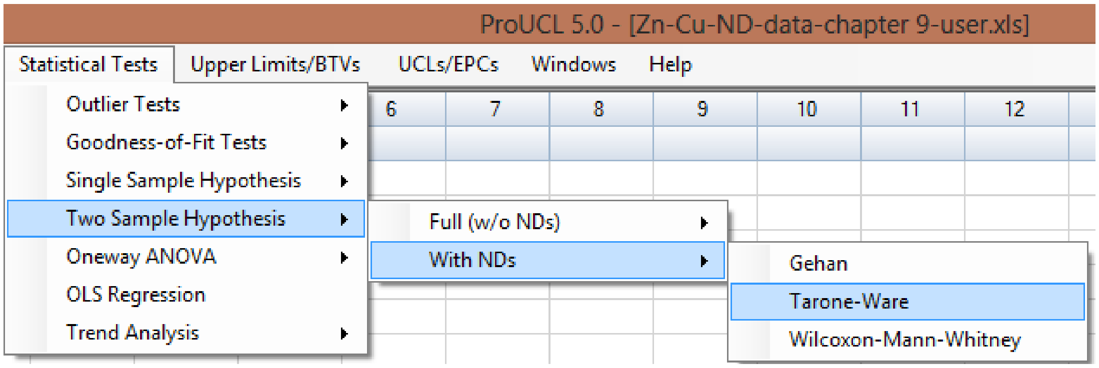
Gehan z Test Value	-3.037
Critical z (0.05)	-1.645
P-Value	0.0012

Conclusion with Alpha = 0.05
Reject H0, Conclude Sample 1 < Sample 2

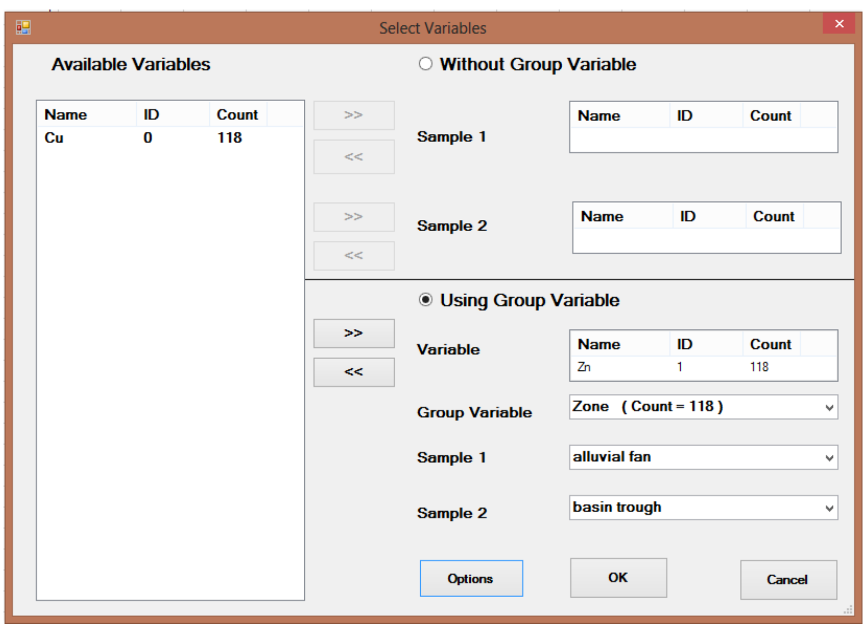
9.2.2.3 Two-Sample Tarone-Ware Test for Data Sets with Nondetects

The two-sample Tarone-Ware (T-W) test (1978) for data sets with NDs is new in ProUCL 5.0.

1. Click **Two Sample Hypothesis Testing ► Two Sample ► With NDs ► Tarone-Ware**



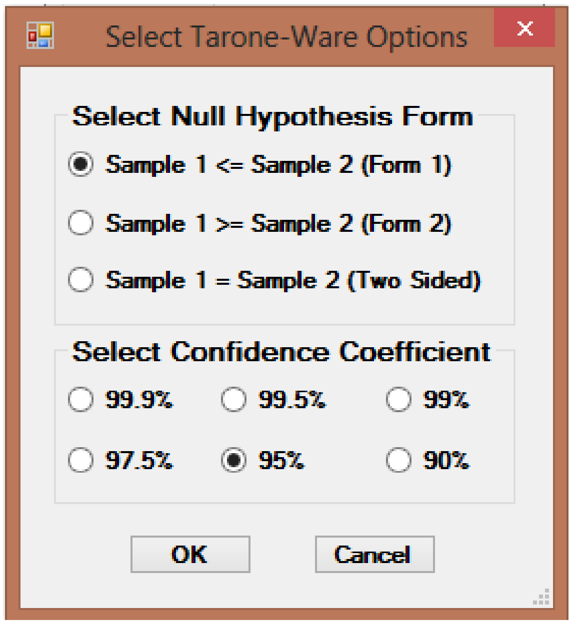
2. The **Select Variables** screen will appear.



- Select variable(s) from the **Select Variables** screen.
- **Without Group Variable**: This option is used when the data values of the variable (Cu) for the two data sets are given in separate columns.
- **With Group Variable**: This option is used when data values of the variable (Cu) for the two data sets are given in the same column. The values are separated into different samples (groups) by the values of an associated **Group Variable**. When using this

option, the user should select a group variable/ID by clicking the arrow next to the **Group Variable** option for a drop-down list of available variables. The user selects an appropriate group variable representing the groups to be tested.

- When the **Options** button is clicked, the following window will be shown.



  - Choose the **Confidence Coefficient**. The default choice is **95%**.
  - Select the form of Null Hypothesis. The default is **Sample 1 <= Sample 2 (Form 1)**.
  - Click on **OK** button to continue or on **Cancel** button to cancel selected options.

- Click on the **OK** button to continue or on the **Cancel** button to cancel the Sample 1 vs. Sample 2 Comparison.

Example 9-6b (continued). Consider the copper and zinc data set used earlier. The data set is used here to illustrate the T-W two-sample test. The output sheet generated by ProUCL 5.0/ProUCL 5.1 is described as follows.

Output for Two-Sample Tarone-Ware Test (with Nondetects)

Confidence Coefficient	95%
Selected Null Hypothesis	Sample 1 Mean/Median <= Sample 2 Mean/Median (Form 1)
Alternative Hypothesis	Sample 1 Mean/Median > Sample 2 Mean/Median

Sample 1 Data: Zn(alluvial fan)
Sample 2 Data: Zn(basin trough)

Raw Statistics

	Sample 1	Sample 2
Number of Valid Data	67	50
Number of Missing Observations	1	0
Number of Non-Detects	16	4
Number of Detects	51	46
Minimum Non-Detect	3	3
Maximum Non-Detect	10	10
Percent Non-detects	23.88%	8.00%
Minimum Detect	5	3
Maximum Detect	620	90
Mean of Detects	27.88	23.13
Median of Detects	11	20
SD of Detects	85.02	19.03

Sample 1 vs Sample 2 Tarone-Ware Test

H0: Mean/Median of Sample 1 <= Mean/Median of Sample 2

TW Statistic	-2.113
TW Critical Value (0.05)	1.645
P-Value	0.983

Conclusion with Alpha = 0.05
Do Not Reject H0, Conclude Sample 1 <= Sample 2
P-Value >= alpha (0.05)

Chapter 10

Computing Upper Limits to Estimate Background Threshold Values Based Upon Full Uncensored Data Sets and Left-Censored Data Sets with Nondetects

This chapter illustrates the computations of parametric and nonparametric statistics and upper limits that can be used as estimates of BTVs and other not-to-exceed values. The BTV estimation methods are available for data sets with and without ND observations. Technical details about the computation of the various limits can be found in the associated ProUCL 5.1 Technical Guide. For each selected variable, this option computes various upper limits such as UPLs, UTLs, USLs and upper percentiles to estimate the BTVs that are used in site versus background evaluations.

Two choices are available to compute background statistics for data sets:

- Full (w/o NDs) – computes background statistics for uncensored full data sets without any ND observation.

- With NDs – computes background statistics for data sets consisting of detected as well as nondetected observations with multiple detection limits.

The user specifies the confidence coefficient (probability) associated with each interval estimate. ProUCL accepts a CC value in the interval [0.5, 1), 0.5 inclusive. The default choice is 0.95. For data sets with and without NDs, ProUCL 5.0/ProUCL 5.1 can compute the following upper limits to estimate BTVs:

- Parametric and nonparametric upper percentiles.

- Parametric and nonparametric UPLs for a single observation, future or next k (≥ 1) observations, mean of next k observations. Here future k, or next k observations may represent k observations from another population (e.g., site) different from the sampled (background) population.

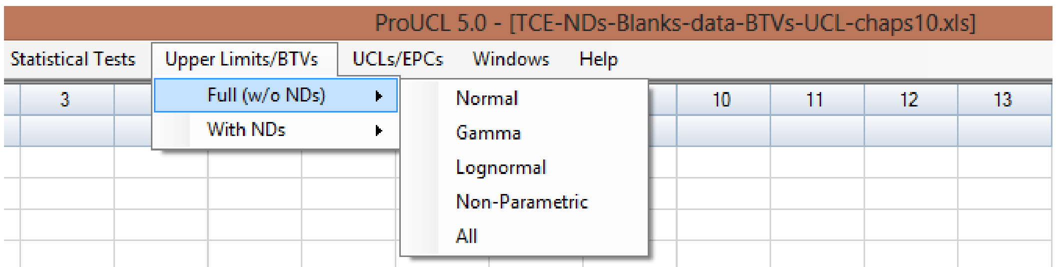
- Parametric and nonparametric UTLs.

- Parametric and nonparametric USLs.

Note on Computing Lower Limits: In many environmental applications (e.g., groundwater monitoring), one needs to compute lower limits including: lower prediction limits (LPLs), lower tolerance limits (LTLs), or lower simultaneous limit (LSLs). At present, ProUCL does not directly compute a LPL, LTL, or a LSL. It should be noted that for data sets with and without nondetects, ProUCL outputs several intermediate results and critical values (e.g., khat, nuhat, K, d2max) needed to compute the interval estimates and lower limits. For data sets with and without NDs, except for the bootstrap methods, the same critical value (e.g., normal z value, Chebyshev critical value, or t-critical value) can be used to compute a parametric LPL, LSL, or a LTL (for samples of size >30 to be able to use Natrella's approximation in LTL) as used in the computation of a UPL, USL, or a UTL (for samples of size >30). Specifically, to compute a LPL, LSL, and LTL (n>30) the '+' sign used in the computation of the corresponding UPL, USL, and UTL (n>30) needs to be replaced by the '-' sign in the equations used to compute UPL, USL, and UTL (n>30). For specific details, the user may want to consult a statistician. For data sets *without ND* observations, the user may want to use the Scout 2008 software package (EPA 2009c) to compute the various parametric and nonparametric LPLs, LTLs (all sample sizes), and LSLs.

10.1 Background Statistics for Full Data Sets without Nondetects

1. Click **Upper Limits/BTVs ► Full (w/o NDs)**



2. Select **Full (w/o NDs)**

- To compute background statistics assuming the normal distribution, click on **Normal** from the drop-down menu list.

- To compute background statistics assuming the gamma distribution, click on **Gamma** from the drop-down menu list.

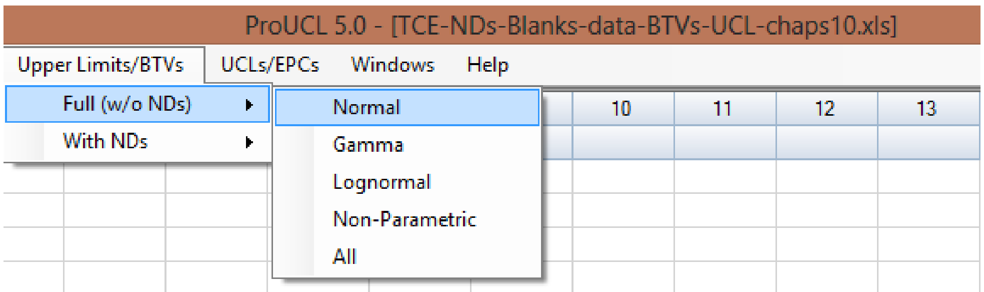
- To compute background statistics assuming the lognormal distribution, click on **Lognormal** from the drop-down menu list.

- To compute background statistics using distribution-free nonparametric methods, click on **Non-Parametric** from the drop-down menu list.

- To compute and see all background statistics available in ProUCL, click on the **All** option from the drop-down menu list. ProUCL will display data distribution, all parametric and nonparametric background statistics in an Excel type spreadsheet. The user may use this output sheet to select the most appropriate statistic to estimate a BTV.

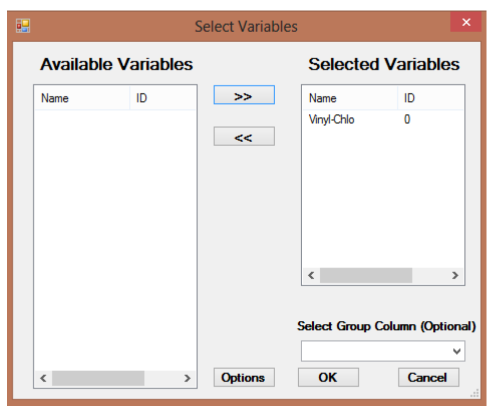
10.1.1 Normal or Lognormal Distribution

1. Click **Upper Limits/BTVs ► Full (w/o NDs) ► Normal or Lognormal**

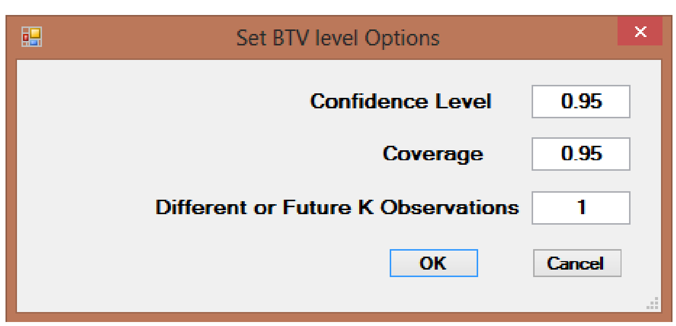


2. The **Select Variables** screen (Chapter 3) will appear.

- Select a variable(s) from the **Select Variables** screen.
- To compute BTV estimates by a group variable, select a group variable by clicking the arrow below the **Select Group Column (Optional)** to obtain a drop-down list of available variables and select an appropriate group variable.



When the **Option** button is clicked, the following window will be shown.



- o Specify the **Confidence Level**; a number in the interval (0.5, 1), 0.5 inclusive. The default choice is **0.95**.

- o Specify the **Coverage** coefficient (for a percentile) needed to compute UTLs. **Coverage** represents a number in the interval (0.0, 1). The default choice is **0.95**. Remember, a UTL is an upper confidence limit (e.g., with confidence level = 0.95) for a 95% (e.g., with coverage = 0.95) percentile.

- o Specify the **Different or Future K Observations**. The default choice is **1**. It is noted that when K = 1, the resulting interval will be a UPL for a single future observation. In the example shown above, a value of K = **1** has been used.

- o Click on **OK** button to continue or on **Cancel** button to cancel this option.

- Click on **OK** to continue or on **Cancel** button to cancel the Upper Limits/BTVs options.

Example 10-1a. Consider the real data set described in Example 1-1 of Chapter 1 collected from a Superfund site. Aluminum concentrations follow a normal distribution and manganese concentrations follow a lognormal distribution. The normal and lognormal distribution based estimates of BTVs are summarized in the following two tables.

Aluminum - Output Screen for BTV Estimates Based upon a Normal Distribution (Full - Uncensored Data Set)

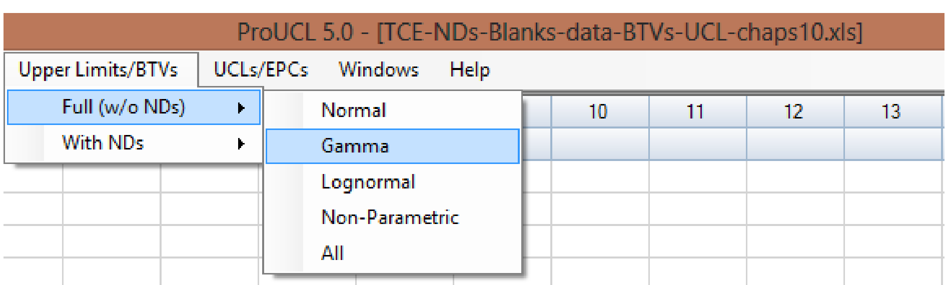
User Selected Options			
Date/Time of Computation	3/18/2013 9:26:21 PM		
From File	SuperFund.xls		
Full Precision	OFF		
Confidence Coefficient	95%		
Coverage	95%		
New or Future K Observations	1		
Aluminum			
General Statistics			
Total Number of Observations	24	Number of Distinct Observations	24
Minimum	1710	First Quartile	4058
Second Largest	15400	Median	7010
Maximum	16200	Third Quartile	10475
Mean	7789	SD	4264
Coefficient of Variation	0.547	Skewness	0.542
Mean of logged Data	8.798	SD of logged Data	0.61
Critical Values for Background Threshold Values (BTVs)			
Tolerance Factor K (For UTL)	2.309	d2max (for USL)	2.644
Normal GOF Test			
Shapiro Wilk Test Statistic	0.939	**Shapiro Wilk GOF Test**	
5% Shapiro Wilk Critical Value	0.916	Data appear Normal at 5% Significance Level	
Lilliefors Test Statistic	0.109	**Lilliefors GOF Test**	
5% Lilliefors Critical Value	0.181	Data appear Normal at 5% Significance Level	
Data appear Normal at 5% Significance Level			
Background Statistics Assuming Normal Distribution			
95% UTL with 95% Coverage	17635	90% Percentile (z)	13254
95% UPL (t)	15248	95% Percentile (z)	14803
95% USL	19063	99% Percentile (z)	17708

Manganese -Output Screen for BTV Estimates Based upon a Lognormal Distribution (Full-Uncensored Data Set)

	Lognormal Background Statistics for Uncensored Full Data Sets		
User Selected Options			
From File	SuperFund.xls		
Full Precision	OFF		
Confidence Coefficient	95%		
Coverage	95%		
New or Future K Observations	1		
Number of Bootstrap Operations	2000		
Manganese			
General Statistics			
Total Number of Observations	24	Number of Distinct Observations	23
Minimum	8.6	First Quartile	29.3
Second Largest	440	Median	71.25
Maximum	530	Third Quartile	122.5
Mean	113.8	SD	134.5
Coefficient of Variation	1.181	Skewness	2.17
Mean of logged Data	4.192	SD of logged Data	1.084
Critical Values for Background Threshold Values (BTVs)			
Tolerance Factor K (For UTL)	2.309	d2max (for USL)	2.644
Lognormal GOF Test			
Shapiro Wilk Test Statistic	0.972	**Shapiro Wilk Lognormal GOF Test**	
5% Shapiro Wilk Critical Value	0.916	Data appear Lognormal at 5% Significance Level	
Lilliefors Test Statistic	0.12	**Lilliefors Lognormal GOF Test**	
5% Lilliefors Critical Value	0.181	Data appear Lognormal at 5% Significance Level	
Data appear Lognormal at 5% Significance Level			
Background Statistics assuming Lognormal Distribution			
95% UTL with 95% Coverage	808.1	90% Percentile (z)	265.4
95% UPL (t)	440.6	95% Percentile (z)	393.5
95% USL	1162	99% Percentile (z)	823.5

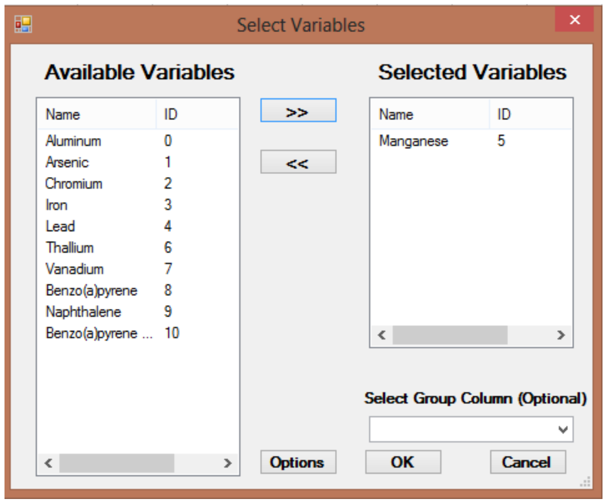
10.1.2 Gamma Distribution

1. Click **Upper Limits/BTVs ► Full (w/o NDs) ► Gamma**



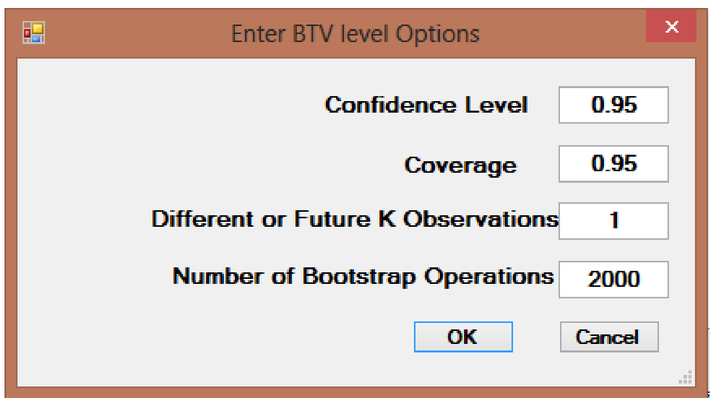
2. The **Select Variables** screen (Chapter 3) will appear.

   - Select a variable(s) from the **Select Variables** screen.



- If needed, select a group variable by clicking the arrow below the **Select Group Column (Optional)** to obtain a drop-down list of variables, and select a proper group variable.

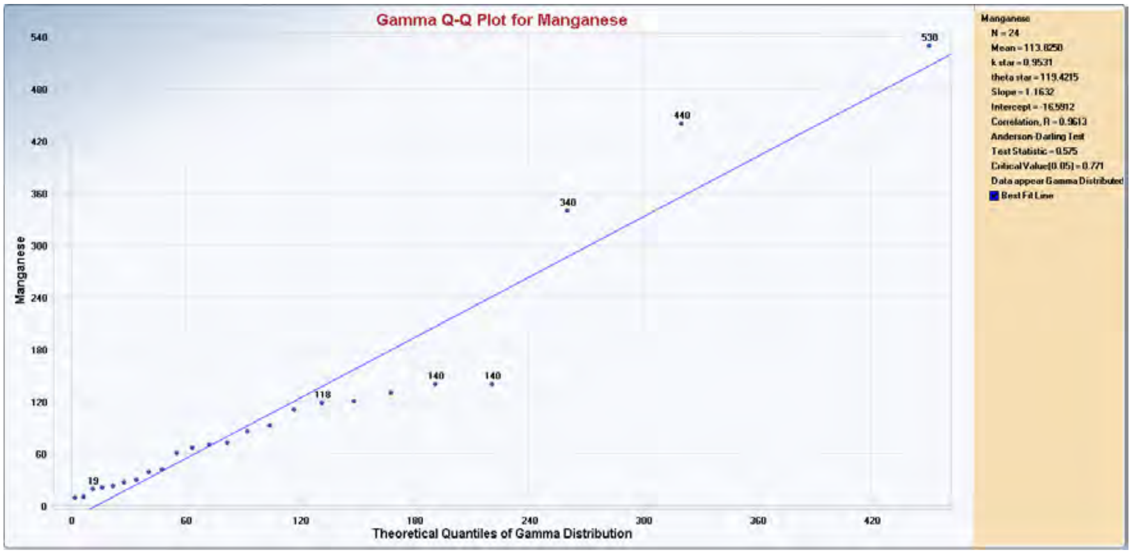
- When the **Option** button is clicked, the following window will be shown.



  - Specify the **Confidence Level**; a number in the interval (0.5, 1), 0.5 inclusive. The default choice is **0.95**.
  - Specify the **Coverage** level; a number in interval (0.0, 1). Default choice is **0.95**.
  - Specify the **Future K.** The default choice is **1.**
  - Specify the **Number of Bootstrap Operations**. The default choice is **2000**.
  - Click on **OK** button to continue or on **Cancel** button to cancel the option.

- Click on **OK** to continue or on **Cancel** button to cancel the Upper Limits/BTVs options.

Example 10-1b (continued). Manganese concentrations also follow a gamma distribution. The gamma distribution based BTV estimates are summarized in the following table generated by ProUCL 5.0. The Gamma GOF test is shown in the following figure.



Gamma GOF Test for Manganese Data Set

Manganese - Output Screen for BTV Estimates Based Upon a Gamma Distribution (Full-Uncensored Data Set)

Manganese			
General Statistics			
Total Number of Observations	24	Number of Distinct Observations	23
Minimum	8.6	First Quartile	29.3
Second Largest	440	Median	71.25
Maximum	530	Third Quartile	122.5
Mean	113.8	SD	134.5
Coefficient of Variation	1.181	Skewness	2.17
Mean of logged Data	4.192	SD of logged Data	1.084
Critical Values for Background Threshold Values (BTVs)			
Tolerance Factor K (For UTL)	2.309	d2max (for USL)	2.644
Gamma GOF Test			
A-D Test Statistic	0.575	**Anderson-Darling Gamma GOF Test**	
5% A-D Critical Value	0.771	Detected data appear Gamma Distributed at 5% Significance Level	
K-S Test Statistic	0.168	**Kolmogrov-Smirnoff Gamma GOF Test**	
5% K-S Critical Value	0.183	Detected data appear Gamma Distributed at 5% Significance Level	
Detected data appear Gamma Distributed at 5% Significance Level			
Gamma Statistics			
k hat (MLE)	1.058	k star (bias corrected MLE)	0.953
Theta hat (MLE)	107.6	Theta star (bias corrected MLE)	119.4
nu hat (MLE)	50.76	nu star (bias corrected)	45.75
MLE Mean (bias corrected)	113.8	MLE Sd (bias corrected)	116.6
Background Statistics Assuming Gamma Distribution			
95% Wilson Hilferty (WH) Approx. Gamma UPL	353.6	90% Percentile	265.2
95% Hawkins Wixley (HW) Approx. Gamma UPL	364.2	95% Percentile	346.8
95% WH Approx. Gamma UTL with 95% Coverage	503.8	99% Percentile	537
95% HW Approx. Gamma UTL with 95% Coverage	540.3		
95% WH USL	611.3	95% HW USL	672.3

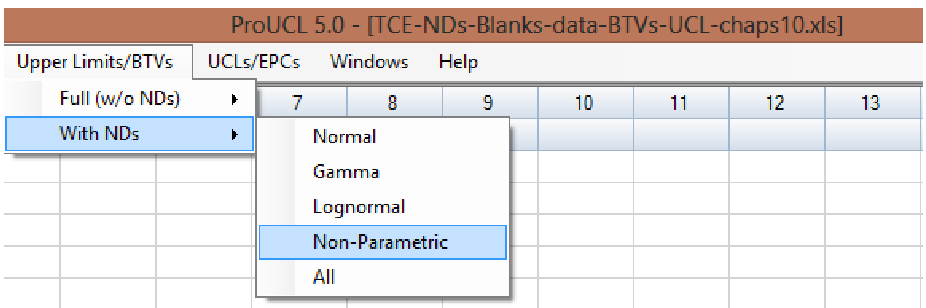
The mean manganese concentration is 113.8 with *sd* = 134.5, and the maximum value = 530. The UTL based upon a lognormal distribution is 808.1 which is significantly higher than the largest value of 530. It is noted that the *sd* of the log-transformed data is 1.084. By comparing BTV estimates computed using lognormal and gamma distributions, it is noted that the lognormal distribution based upper limits, UTL and UPL, are significantly higher than those based upon a gamma distribution confirming the statements made earlier that the use of a lognormal distribution tends to yield inflated values of the upper limits used to estimate environmental parameters (e.g., BTVs, EPCs). These upper limits are summarized as follows.

	Lognormal	**Gamma (WH)**	**Gamma (HW)**
UTL95-95	808.1	504	540.3
UPL95	440.6	353.6	364.2

Mean = 113.8, Max value = 530.

10.1.3 Nonparametric Methods

1. Click **Upper Limits/BTVs ► Full (w/o NDs) ► Non-Parametric**

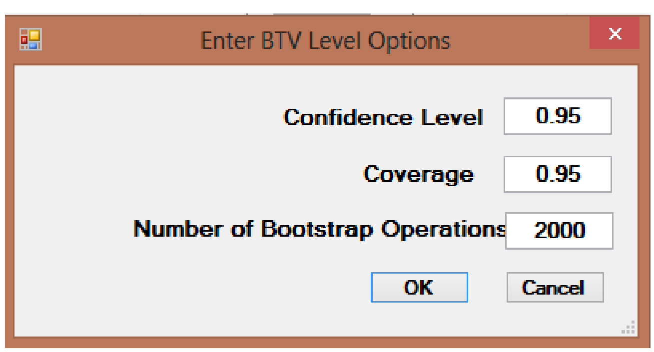


2. The **Select Variables** screen (Chapter 3) will appear.

- Select a variable(s) from the **Select Variables** screen.

- If needed, select a group variable by clicking the arrow below the **Select Group Column (Optional)** to obtain a drop-down list of variables, and select a proper group variable.

- When the **Option** button is clicked, the following window will be shown.



- Specify the **Confidence Level**; a number in the interval (0.5, 1), 0.5 inclusive. The default choice is **0.95**.
- Specify the **Coverage** level; a number in the interval (0.0, 1). Default choice is **0.95**.
- Specify the **Number of Bootstrap Operations**. The default choice is **2000**.
- Click on the **OK** button to continue or on the **Cancel** button to cancel the option.

- Click **OK** button to continue or **Cancel** button to cancel the Upper Limits/BTVs options.

Example 10-2. Lead concentrations data set used in Example 1-1 does not follow a discernible distribution. Nonparametric BTV estimates are summarized as follows. ProUCL 5.1 also outputs the sample size needed to compute a nonparametric UTL needed to achieve the specified CC.

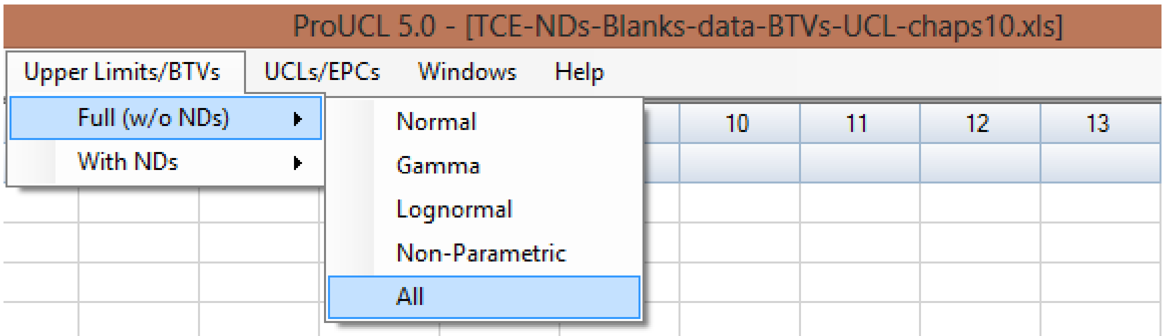
Lead - Output Screen for Nonparametric BTVs Estimates (Full-Uncensored Data Set)

General Statistics			
Total Number of Observations	24	Number of Distinct Observations	18
Minimum	4.9	First Quartile	10.43
Second Largest	98.5	Median	14
Maximum	109	Third Quartile	19.25
Mean	22.49	SD	26.83
Coefficient of Variation	1.193	Skewness	2.665
Mean of logged Data	2.743	SD of logged Data	0.771
Critical Values for Background Threshold Values (BTVs)			
Tolerance Factor K (For UTL)	2.309	d2max (for USL)	2.644
Nonparametric Distribution Free Background Statistics			
Data do not follow a Discernible Distribution (0.05)			
Nonparametric Upper Limits for Background Threshold Values			
Order of Statistic, r	24	95% UTL with 95% Coverage	109
Approximate f	1.263	Approximate Actual Confidence Coefficient achieved by UTL	0.708
		Approximate Sample Size needed to achieve specified CC	59
95% Percentile Bootstrap UTL with 95% Coverage	109	95% BCA Bootstrap UTL with 95% Coverage	109
95% UPL	106.4	90% Percentile	44.81
90% Chebyshev UPL	104.6	95% Percentile	91.72
95% Chebyshev UPL	141.8	99% Percentile	106.6

To compute nonparametric upper limits providing the specified coverage (e.g., 0.95), sizes of the data sets should be fairly large (e.g., > 59). For details, consult the associated ProUCL Technical Guide. In this example the sample size is only 24, and the confidence coefficient (CC) achieved by the nonparametric, UTL is only 0.71 which is significantly lower than the desired CC of 0.95.

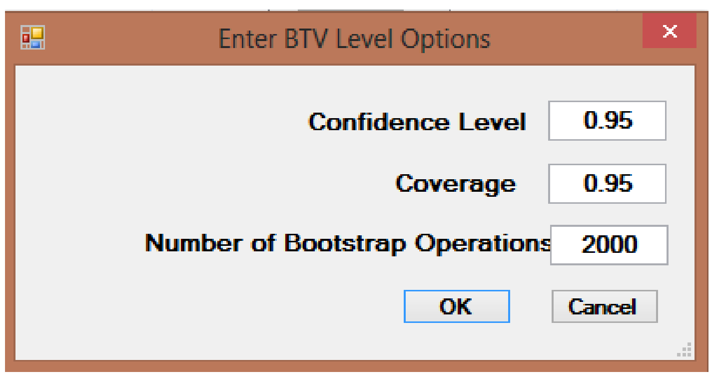
10.1.4 All Statistics Option

1. Click **Upper Limits/BTVs ► Full (w/o NDs) ► All**



2. The **Select Variables** screen (Chapter 3) will appear.

- Select a variable(s) from the **Select Variables** screen.
- If needed, select a group variable by clicking the arrow below the **Select Group Column (Optional)** to obtain a drop-down list of variables, and select a proper group variable.
- When the **Option** button is clicked, the following window will be shown.



  - Specify the **Confidence Level**; a number in the interval (0.5, 1), 0.5 inclusive. The default choice is **0.95**.
  - Specify the **Coverage** level; a number in the interval (0.0, 1). Default is **0.9**.
  - Specify the **Future K**. The default choice is **1**.
  - Specify the **Number of Bootstrap Operations**. The default choice is **2000.**
  - Click on **OK** button to continue or on **Cancel** button to cancel the option.

- Click on **OK** to continue or on **Cancel** button to cancel the Upper Limits/BTVs options.

Example 10-1c (continued). The various BTV estimates based upon the manganese concentrations computed using the **All** option of ProUCL are summarized as follows. The **All** option computes and displays all available parametric and nonparametric BTV estimates. This option also informs the user about the distribution(s) of the data set. This option is specifically useful when one has to process many analytes (variables) without any knowledge about their probability distributions.

Manganese - Output Screen for All BTVs Estimates (Full-Uncensored Data Set)

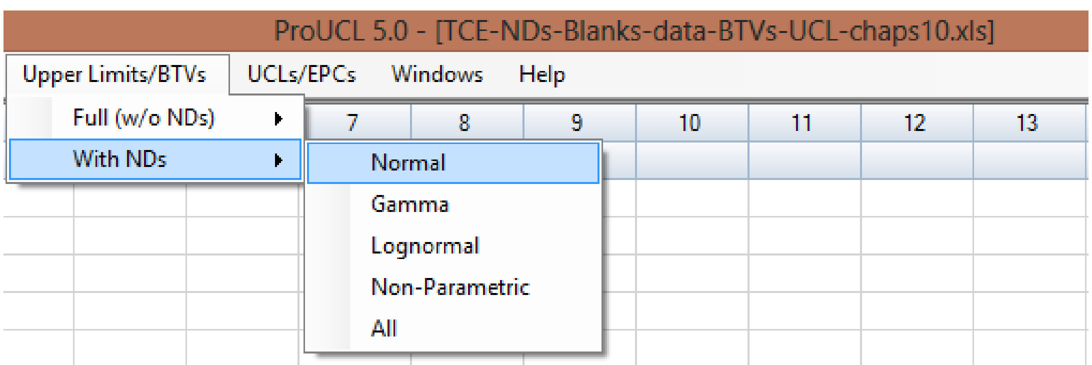
Manganese			
General Statistics			
Total Number of Observations	24	Number of Distinct Observations	23
Minimum	8.6	First Quartile	29.3
Second Largest	440	Median	71.25
Maximum	530	Third Quartile	122.5
Mean	113.8	SD	134.5
Coefficient of Variation	1.181	Skewness	2.17
Mean of logged Data	4.192	SD of logged Data	1.084
Critical Values for Background Threshold Values (BTVs)			
Tolerance Factor K (For UTL)	2.309	d2max (for USL)	2.644
Normal GOF Test			
Shapiro Wilk Test Statistic	0.697	**Shapiro Wilk GOF Test**	
5% Shapiro Wilk Critical Value	0.916	Data Not Normal at 5% Significance Level	
Lilliefors Test Statistic	0.298	**Lilliefors GOF Test**	
5% Lilliefors Critical Value	0.181	Data Not Normal at 5% Significance Level	
Data Not Normal at 5% Significance Level			
Background Statistics Assuming Normal Distribution			
95% UTL with 95% Coverage	424.3	90% Percentile (z)	286.1
95% UPL (t)	349	95% Percentile (z)	335
95% USL	469.3	99% Percentile (z)	426.6
Gamma GOF Test			
A-D Test Statistic	0.575	**Anderson-Darling Gamma GOF Test**	
5% A-D Critical Value	0.771	Detected data appear Gamma Distributed at 5% Significance Level	
K-S Test Statistic	0.168	**Kolmogrov-Smirnoff Gamma GOF Test**	
5% K-S Critical Value	0.183	Detected data appear Gamma Distributed at 5% Significance Level	
Detected data appear Gamma Distributed at 5% Significance Level			
Gamma Statistics			
k hat (MLE)	1.058	k star (bias corrected MLE)	0.953
Theta hat (MLE)	107.6	Theta star (bias corrected MLE)	119.4
nu hat (MLE)	50.76	nu star (bias corrected)	45.75
MLE Mean (bias corrected)	113.8	MLE Sd (bias corrected)	116.6
Background Statistics Assuming Gamma Distribution			
95% Wilson Hilferty (WH) Approx. Gamma UPL	353.6	90% Percentile	265.2
95% Hawkins Wixley (HW) Approx. Gamma UPL	364.2	95% Percentile	346.8
95% WH Approx. Gamma UTL with 95% Coverage	503.8	99% Percentile	537
95% HW Approx. Gamma UTL with 95% Coverage	540.3		
95% WH USL	611.3	95% HW USL	672.3

Manganese - Output Screen for All BTVs Estimates - Continued
(Full-Uncensored Data Set)

Lognormal GOF Test			
Shapiro Wilk Test Statistic	0.972	**Shapiro Wilk Lognormal GOF Test**	
5% Shapiro Wilk Critical Value	0.916	Data appear Lognormal at 5% Significance Level	
Lilliefors Test Statistic	0.12	**Lilliefors Lognormal GOF Test**	
5% Lilliefors Critical Value	0.181	Data appear Lognormal at 5% Significance Level	
Data appear Lognormal at 5% Significance Level			
Background Statistics assuming Lognormal Distribution			
95% UTL with 95% Coverage	808.1	90% Percentile (z)	265.4
95% UPL (t)	440.6	95% Percentile (z)	393.5
95% USL	1162	99% Percentile (z)	823.5
Nonparametric Distribution Free Background Statistics			
Data appear Gamma Distributed at 5% Significance Level			
Nonparametric Upper Limits for Background Threshold Values			
Order of Statistic, r	24	95% UTL with 95% Coverage	530
Approximate f	1.263	Confidence Coefficient (CC) achieved by UTL	0.708
95% Percentile Bootstrap UTL with 95% Coverage	530	95% BCA Bootstrap UTL with 95% Coverage	530
95% UPL	507.5	90% Percentile	280
90% Chebyshev UPL	525.5	95% Percentile	425
95% Chebyshev UPL	712	99% Percentile	509.3
95% USL	530		

10.2 Background Statistics with NDs

1. Click **Upper Limits/BTVs ► With NDs**



2. Select the **With NDs** option.

- To compute background statistics assuming the normal distribution, click on **Normal** from the drop-down menu list.

- To compute background statistics assuming the gamma distribution, click on **Gamma** from the drop-down menu list.

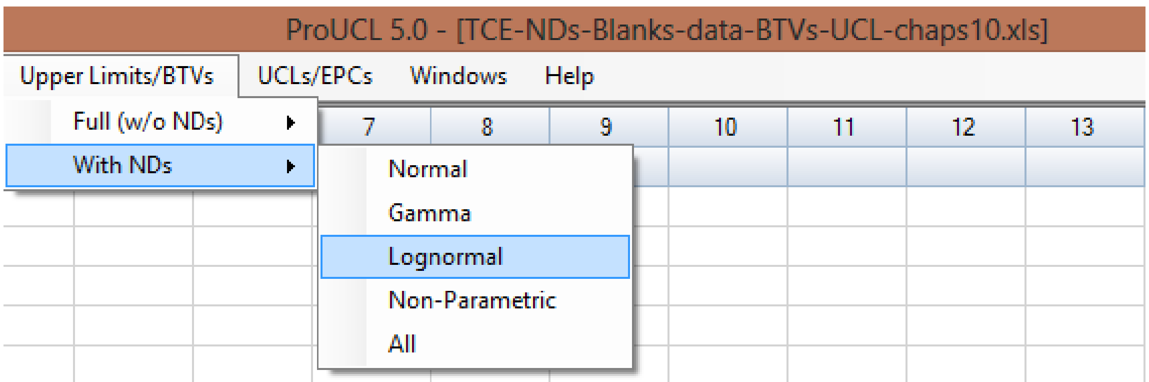
- To compute background statistics assuming the lognormal distribution, click on **Lognormal** from the drop-down menu list.

- To compute background statistics using distribution-free methods, click on **Non-Parametric** from the drop-down menu list.

- To compute all available background statistics in ProUCL, click on the **All** option from the drop-down menu list.

10.2.1 Normal or Lognormal Distribution

1. Click **Upper Limits/BTVs ► With NDs ► Normal or Lognormal**

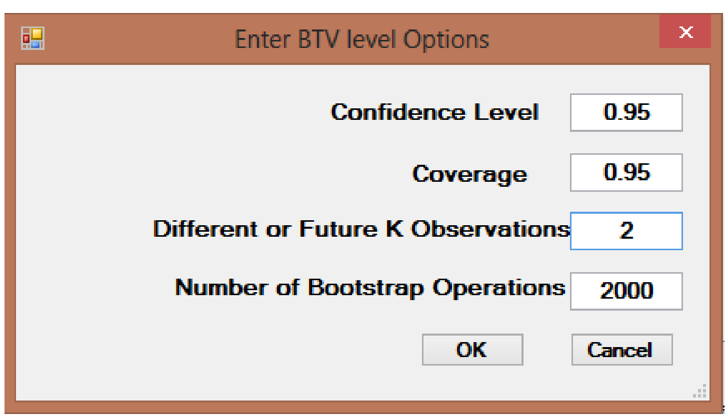


2. The **Select Variables** screen (Chapter 3) will appear.

    - Select a variable(s) from the **Select Variables** screen.

    - If needed, select a group variable by clicking the arrow below the **Select Group Column (Optional)** to obtain a drop-down list of variables, and select a proper group variable.

    - When the option button is clicked, the following window will be shown.



    - Specify the **Confidence Level**; a number in the interval (0.5, 1), 0.5 inclusive. The default choice is **0.95**.

- Specify the **Coverage** level; a number in the interval (0.0, 1). Default choice is **0.95**.
- Specify the **Future K**. The default choice is **1**.
- Specify the **Number of Bootstrap Operations.** The default choice is **2000.**
- Click on the **OK** button to continue or on the **Cancel** button to cancel the option.

- Click on **OK** to continue or on **Cancel** button to cancel the Upper limits/BTVs options.

Example 10-3a. Consider a small real TCE data set of size n=12 consisting of 4 ND observations. The detected data set of size 8 follows a normal as well as a lognormal distribution. The BTV estimates using the LROS method, normal and lognormal distribution on KM estimates, and nonparametric Chebyshev inequality and bootstrap methods on KM estimates are summarized in the following two tables. It is noted that upper limits including UTL95-95 and UPL95 based upon the robust LROS method yield much higher values than the other methods including KM estimates in normal and lognormal equations to compute the upper limits. It is noted that the detected data also follows a gamma distribution. The gamma distribution (of detected data) based BTV estimates are described in the next section.

TCE - Output Screen for BTV Estimates Computed Using Normal Distribution of Detected Data (Left-Censored Data Set with NDs)

User Selected Options	
From File	TCE-NDs-Blanks-data-BTVs-UCL-chaps.xls
Full Precision	OFF
Confidence Coefficient	95%
Coverage	95%
Different or Future K Observations	2

TCE

General Statistics			
Total Number of Observations	12	Number of Distinct Observations	9
Number of Missing Observations	2		
Number of Detects	8	Number of Non-Detects	4
Number of Distinct Detects	8	Number of Distinct Non-Detects	1
Minimum Detect	0.75	Minimum Non-Detect	0.68
Maximum Detect	9.29	Maximum Non-Detect	0.68
Variance Detected	9.732	Percent Non-Detects	33.33%
Mean Detected	2.941	SD Detected	3.12
Mean of Detected Logged Data	0.634	SD of Detected Logged Data	0.978
Critical Values for Background Threshold Values (BTVs)			
Tolerance Factor K (For UTL)	2.736	d2max (for USL)	2.285
Normal GOF Test on Detects Only			
Shapiro Wilk Test Statistic	0.765	**Shapiro Wilk GOF Test**	
5% Shapiro Wilk Critical Value	0.818	Data Not Normal at 5% Significance Level	
Lilliefors Test Statistic	0.256	**Lilliefors GOF Test**	
5% Lilliefors Critical Value	0.313	Detected Data appear Normal at 5% Significance Level	
Detected Data appear Approximate Normal at 5% Significance Level			

TCE (continued) - Output Screen for BTV Estimates Computed Using Normal Distribution of Detected Data (Left-Censored Data Set with NDs)

Kaplan Meier (KM) Background Statistics Assuming Normal Distribution			
Mean	2.188	SD	2.61
95% UTL95% Coverage	9.329	95% KM UPL (t)	7.067
95% KM UPL for Next 2 Observations	8.167	95% KM UPL for Mean of Next 2 Observations	5.768
95% KM Chebyshev UPL	14.03	90% KM Percentile (z)	5.533
95% KM Percentile (z)	6.481	99% KM Percentile (z)	8.26

Output Screen for BTV Estimates Computed Using a Lognormal Distribution of Detected Data (Left-Censored Data Set with NDs)

	Lognormal Background Statistics for Data Sets with Non-Detects		
User Selected Options			
From File	TCE-NDs-Blanks-data-BTVs-UCL-chaps10.xls		
Full Precision	OFF		
Confidence Coefficient	95%		
Coverage	95%		
Different or Future K Observations	2		
Number of Bootstrap Operations	2000		
TCE			
General Statistics			
Total Number of Observations	12	Number of Distinct Observations	9
Number of Missing Observations	2		
Number of Detects	8	Number of Non-Detects	4
Number of Distinct Detects	8	Number of Distinct Non-Detects	1
Minimum Detect	0.75	Minimum Non-Detect	0.68
Maximum Detect	9.29	Maximum Non-Detect	0.68
Variance Detected	9.732	Percent Non-Detects	33.33%
Mean Detected	2.941	SD Detected	3.12
Mean of Detected Logged Data	0.634	SD of Detected Logged Data	0.978
Critical Values for Background Threshold Values (BTVs)			
Tolerance Factor K (For UTL)	2.736	d2max (for USL)	2.285
Lognormal GOF Test on Detected Observations Only			
Shapiro Wilk Test Statistic	0.865	**Shapiro Wilk GOF Test**	
5% Shapiro Wilk Critical Value	0.818	Detected Data appear Lognormal at 5% Significance Level	
Lilliefors Test Statistic	0.258	**Lilliefors GOF Test**	
5% Lilliefors Critical Value	0.313	Detected Data appear Lognormal at 5% Significance Level	
Detected Data appear Lognormal at 5% Significance Level			

Continued: Output Screen for BTV Estimates Computed Using a Lognormal Distribution of Detected Data (Left-Censored Data Set with NDs)

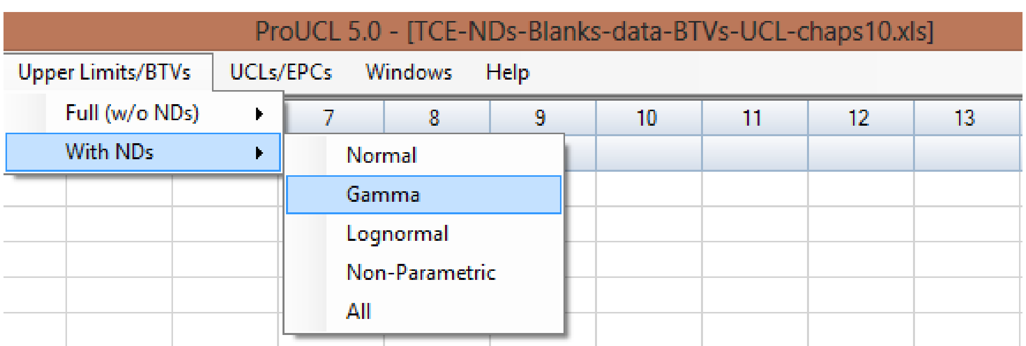
Kaplan Meier (KM) Background Statistics Assuming Normal Distribution			
Mean	2.188	SD	2.61
95% UTL95% Coverage	9.329	95% KM UPL (t)	7.067
95% KM UPL for Next 2 Observations	8.167	95% KM UPL for Mean of Next 2 Observations	5.768
95% KM Chebyshev UPL	14.03	90% KM Percentile (z)	5.533
95% KM Percentile (z)	6.481	99% KM Percentile (z)	8.26
95% KM USL	8.152		

Background Lognormal ROS Statistics Assuming Lognormal Distribution Using Imputed Non-Detects			
Mean in Original Scale	2.018	Mean in Log Scale	-0.214
SD in Original Scale	2.838	SD in Log Scale	1.512
95% UTL95% Coverage	50.54	95% BCA UTL95% Coverage	9.29
95% Bootstrap (%) UTL95% Coverage	9.29	95% UPL (t)	13.63
95% UPL for Next 2 Observations	25.78	95% UPL for Mean of 2 Observations	6.424
90% Percentile (z)	5.606	95% Percentile (z)	9.71
99% Percentile (z)	27.2	95% USL	25.55

Statistics using KM estimates on Logged Data and Assuming Lognormal Distribution			
KM Mean of Logged Data	0.294	95% KM UTL (Lognormal)95% Coverage	15.25
KM SD of Logged Data	0.888	95% KM UPL (Lognormal)	7.06
95% KM Percentile Lognormal (z)	5.784	95% KM USL (Lognormal)	10.21

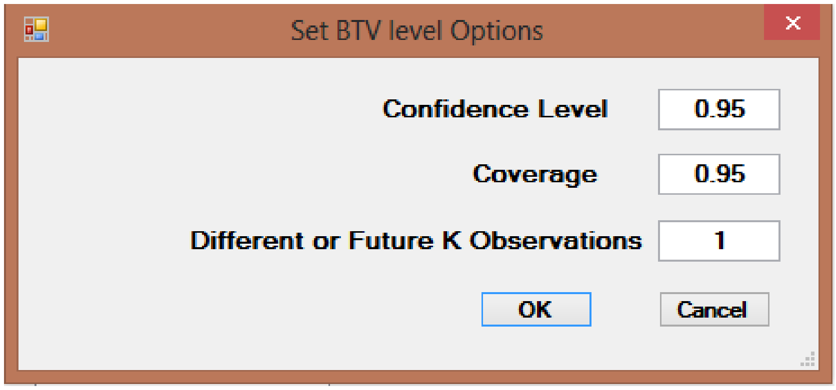
10.2.2 Gamma Distribution

1. Click **Upper Limits/BTVs ► With NDs ► Gamma**



2. The **Select Variables** screen (Chapter 3) will appear.

   - Select a variable(s) from the **Select Variables** screen.
   - If needed, select a group variable by clicking the arrow below the **Select Group Column (Optional)** to obtain a drop-down list of variables, and select a proper group variable.
   - When the **Option** button is clicked, the following window will be shown.



- Specify the **Confidence Level**; a number in the interval (0.5, 1), 0.5 inclusive. The default choice is **0.95**.

- Specify the **Coverage** level; a number in the interval (0.0, 1). Default choice is **0.95**.

- Click on the **OK** button to continue or on the **Cancel** button to cancel option.

- Click on **OK** to continue or on **Cancel** button to cancel the **Upper Limits/BTVs** options.

Example 10-3b (continued). It is noted that the detected TCE data considered in Example 10-3 also follows a gamma distribution. The gamma distribution based upper limits are summarized as follows.

TCE - Output Screen for BTV Estimates Computed Using Gamma Distribution of Detected Data (Left-Censored Data Set with NDs)

TCE			
General Statistics			
Total Number of Observations	12	Number of Distinct Observations	9
Number of Missing Observations	2		
Number of Detects	8	Number of Non-Detects	4
Number of Distinct Detects	8	Number of Distinct Non-Detects	1
Minimum Detect	0.75	Minimum Non-Detect	0.68
Maximum Detect	9.29	Maximum Non-Detect	0.68
Variance Detected	9.732	Percent Non-Detects	33.33%
Mean Detected	2.941	SD Detected	3.12
Mean of Detected Logged Data	0.634	SD of Detected Logged Data	0.978
Critical Values for Background Threshold Values (BTVs)			
Tolerance Factor K (For UTL)	2.736	d2max (for USL)	2.285
Gamma GOF Tests on Detected Observations Only			
A-D Test Statistic	0.624	**Anderson-Darling GOF Test**	
5% A-D Critical Value	0.732	Detected data appear Gamma Distributed at 5% Significance Level	
K-S Test Statistic	0.274	**Kolmogorov-Smirnov GOF**	
5% K-S Critical Value	0.3	Detected data appear Gamma Distributed at 5% Significance Level	
Detected data appear Gamma Distributed at 5% Significance Level			

TCE (continued) - Output Screen for BTV Estimates Computed Using Gamma Distribution of Detected Data (Left-Censored Data Set with NDs)

Gamma Statistics on Detected Data Only			
k hat (MLE)	1.265	k star (bias corrected MLE)	0.874
Theta hat (MLE)	2.326	Theta star (bias corrected MLE)	3.366
nu hat (MLE)	20.23	nu star (bias corrected)	13.98
MLE Mean (bias corrected)	2.941		
MLE Sd (bias corrected)	3.147	95% Percentile of Chisquare (2k)	5.492
Gamma ROS Statistics using Imputed Non-Detects			
Minimum	0.01	Mean	1.964
Maximum	9.29	Median	0.845
SD	2.877	CV	1.465
k hat (MLE)	0.372	k star (bias corrected MLE)	0.335
Theta hat (MLE)	5.274	Theta star (bias corrected MLE)	5.865
nu hat (MLE)	8.938	nu star (bias corrected)	8.037
MLE Mean (bias corrected)	1.964	MLE Sd (bias corrected)	3.394
95% Percentile of Chisquare (2k)	2.956	90% Percentile	5.709
95% Percentile	8.668	99% Percentile	16.26

The following statistics are computed using Gamma ROS Statistics on Imputed Data					
Upper Limits using Wilson Hilferty (WH) and Hawkins Wixley (HW) Methods					
	WH	HW		WH	HW
95% Approx. Gamma UTL with 95% Coverage	19.62	27.19	95% Approx. Gamma UPL	9.793	11.66
95% Gamma USL	13.95	17.89			

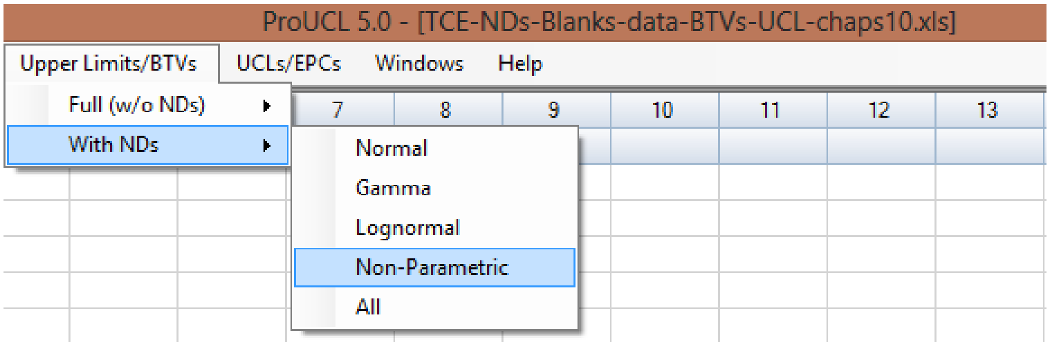
Estimates of Gamma Parameters using KM Estimates			
Mean (KM)	2.188	SD (KM)	2.61
Variance (KM)	6.813	SE of Mean (KM)	0.806
k hat (KM)	0.702	k star (KM)	0.582
nu hat (KM)	13.98	nu star (KM)	13.98
theta hat (KM)	3.115	theta star (KM)	3.757
80% gamma percentile (KM)	3.606	90% gamma percentile (KM)	5.728
95% gamma percentile (KM)	7.957	99% gamma percentile (KM)	13.36

The following statistics are computed using gamma distribution and KM estimates					
Upper Limits using Wilson Hilferty (WH) and Hawkins Wixley (HW) Methods					
	WH	HW		WH	HW
95% Approx. Gamma UTL with 95% Coverage	11.34	11.95	95% Approx. Gamma UPL	6.88	6.896
95% KM Gamma Percentile	5.955	5.902	95% Gamma USL	8.836	9.063

The detected data set does not follow a normal distribution based upon the S-W test, but follows a normal distribution based upon the Lilliefors test. Since the detected data set is of small size (=8), the normal GOF conclusion is suspect. The detected data follow a gamma distribution. There are several NDs reported with a low detection limit of 0.68, therefore, GROS method may yield infeasible negative imputed values. Therefore, the use of a gamma distribution on KM estimates is preferred for computing the BTV estimates. The gamma KM UTL95-95 (HW) =11.34, and gamma KM UTL95-95 (WH) = 11.95. Any one of these two limits can be used to estimate the BTV.

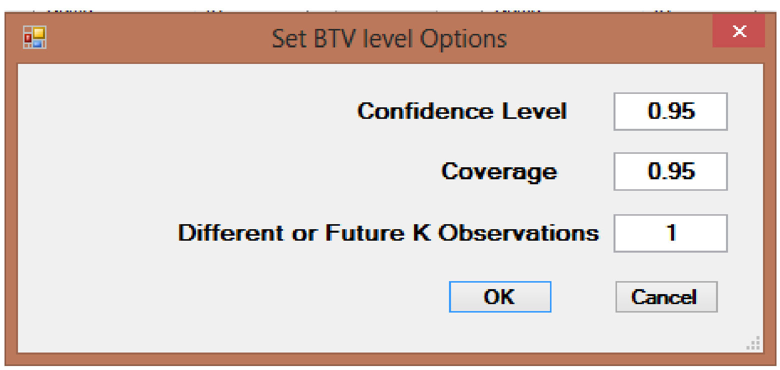
10.2.3 Nonparametric Methods (with NDs)

1. Click **Upper Limits/BTVs► With NDs ► Non-Parametric**



2. The **Select Variables** screen (Chapter 3) will appear.

- Select a variable(s) from the **Select Variables** screen.
- If needed, select a group variable by clicking the arrow below the **Select Group Column (Optional)** to obtain a drop-down list of variables, and select a proper group variable.
- When the **Option** button is clicked, the following window will be shown.



  - Specify the **Confidence Level**; a number in the interval (0.5, 1), 0.5 inclusive. The default choice is **0.95**.
  - Specify the **Coverage** level; a number in interval (0.0, 1). Default choice is **0.95**.
  - Click on the **OK** button to continue or on the **Cancel** button to cancel the option.

- Click on **OK** to continue or on **Cancel** button to cancel the Upper Limit/BTVs option.

Example 10-3c (continued). The nonparametric upper limits based the TCE data considered in Example 10-3 are summarized in the following table.

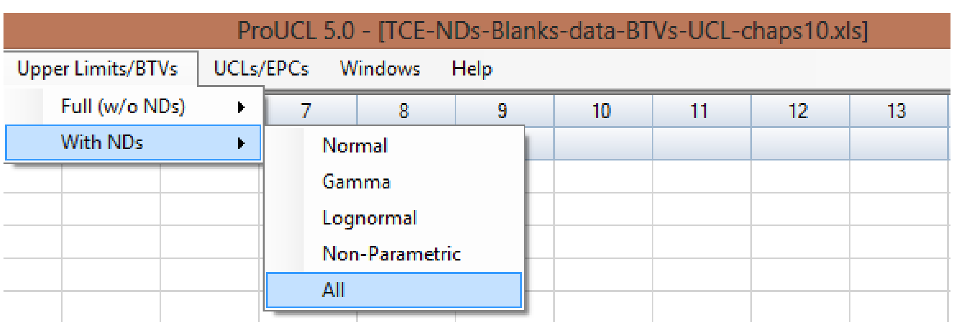
TCE - Output Screen for Nonparametric BTV Estimates
(Left-Censored Data Set with NDs)

TCE

General Statistics			
Total Number of Observations	12	Number of Distinct Observations	9
Number of Missing Observations	2		
Number of Detects	8	Number of Non-Detects	4
Number of Distinct Detects	8	Number of Distinct Non-Detects	1
Minimum Detect	0.75	Minimum Non-Detect	0.68
Maximum Detect	9.29	Maximum Non-Detect	0.68
Variance Detected	9.732	Percent Non-Detects	33.33%
Mean Detected	2.941	SD Detected	3.12
Mean of Detected Logged Data	0.634	SD of Detected Logged Data	0.978
Critical Values for Background Threshold Values (BTVs)			
Tolerance Factor K (For UTL)	2.736	d2max (for USL)	2.285
Nonparametric Distribution Free Background Statistics			
Data appear to follow a Discernible Distribution at 5% Significance Level			
Kaplan Meier (KM) Background Statistics Assuming Normal Distribution			
Mean	2.188	SD	2.61
95% UTL95% Coverage	9.329	95% KM UPL (t)	7.067
95% KM Chebyshev UPL	14.03	90% KM Percentile (z)	5.533
95% KM Percentile (z)	6.481	99% KM Percentile (z)	8.26
95% KM USL	8.152		
Nonparametric Upper Limits for BTVs(no distinction made between detects and nondetects)			
Order of Statistic, r	12	95% UTL with95% Coverage	9.29
Approximate f	0.632	Approximate Actual Confidence Coefficient achieved by UTL	0.46
Approximate Sample Size needed to achieve specified CC	59	95% UPL	9.29
95% USL	9.29	95% KM Chebyshev UPL	14.03

10.2.4 All Statistics Option

1. Click **Upper Limits/BTVs ► With NDs ► All**

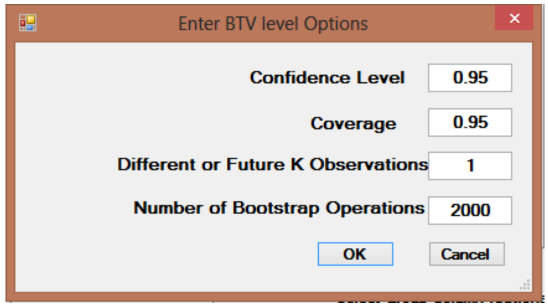


2. The **Select Variables** screen (Chapter 3) will appear.

- Select a variable(s) from the **Select Variables** screen.

- If needed, select a group variable by clicking the arrow below the **Select Group Column (Optional)** to obtain a drop-down list of variables, and select a proper group variable.

- When the **Option** button is clicked, the following window will be shown.



  - Specify the **Confidence Level**; a number in the interval (0.5, 1), 0.5 inclusive. The default choice is **0.95**.

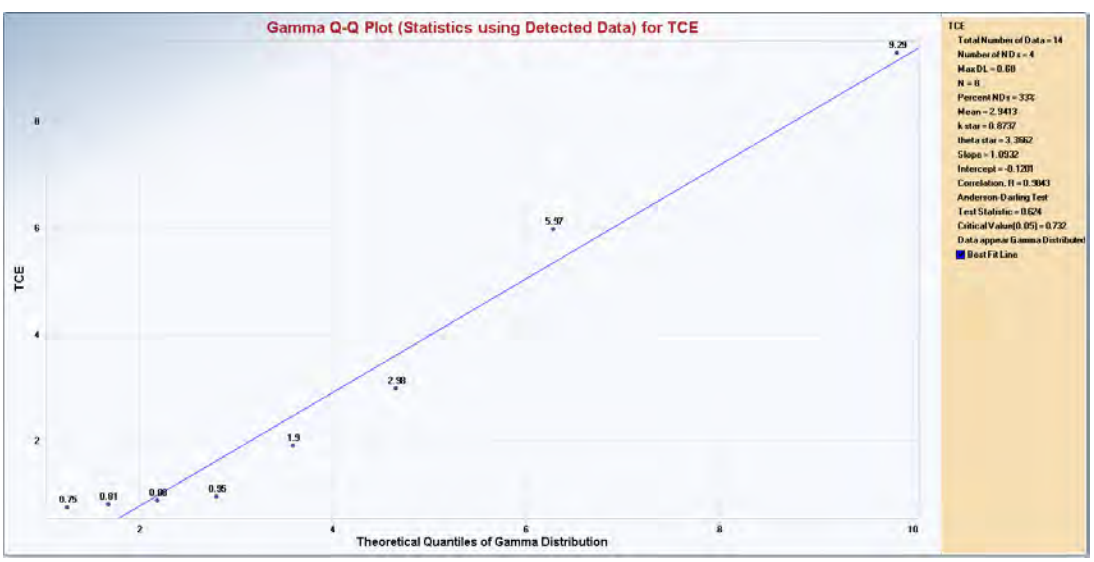
  - Specify the **Coverage** level; a number in the interval (0.0, 1). Default choice is **0.95**.

  - Specify the **Future K**. The default choice is **1**.

  - Click on the **OK** button to continue or on the **Cancel** button to cancel the option.

- Click on **OK** to continue or on **Cancel** button to cancel the Upper Limits/BTVs option.

Example 10-3d (continued). BTV estimates using the **All** option for the TCE data are summarized as follows. The detected data set is of small size (n=8) and follows a gamma distribution. The gamma GOF Q-Q plot based upon detected data is shown in the following figure. The relevant statistics have been high-lighted in the output table provided after the gamma GOF Q-Q plot.



TCE - Output Screen for All BTV Estimates (Left-Censored Data Set with NDs)

TCE			
General Statistics			
Total Number of Observations	12	Number of Missing Observations	2
Number of Distinct Observations	9		
Number of Detects	8	Number of Non-Detects	4
Number of Distinct Detects	8	Number of Distinct Non-Detects	1
Minimum Detect	0.75	Minimum Non-Detect	0.68
Maximum Detect	9.29	Maximum Non-Detect	0.68
Variance Detected	9.732	Percent Non-Detects	33.33%
Mean Detected	2.941	SD Detected	3.12
Mean of Detected Logged Data	0.634	SD of Detected Logged Data	0.978
Critical Values for Background Threshold Values (BTVs)			
Tolerance Factor K (For UTL)	2.736	d2max (for USL)	2.285
Normal GOF Test on Detects Only			
Shapiro Wilk Test Statistic	0.765	Shapiro Wilk GOF Test	
5% Shapiro Wilk Critical Value	0.818	Data Not Normal at 5% Significance Level	
Lilliefors Test Statistic	0.256	Lilliefors GOF Test	
5% Lilliefors Critical Value	0.313	Detected Data appear Normal at 5% Significance Level	
Detected Data appear Approximate Normal at 5% Significance Level			
Kaplan Meier (KM) Background Statistics Assuming Normal Distribution			
Mean	2.188	SD	2.61
95% UTL95% Coverage	9.329	95% KM UPL (t)	7.067
95% KM Chebyshev UPL	14.03	90% KM Percentile (z)	5.533
95% KM Percentile (z)	6.481	99% KM Percentile (z)	8.26
95% KM USL	8.152		
Gamma GOF Tests on Detected Observations Only			
A-D Test Statistic	0.624	Anderson-Darling GOF Test	
5% A-D Critical Value	0.732	Detected data appear Gamma Distributed at 5% Significance Level	
K-S Test Statistic	0.274	Kolmogrov-Smirnoff GOF	
5% K-S Critical Value	0.3	Detected data appear Gamma Distributed at 5% Significance Level	
Detected data appear Gamma Distributed at 5% Significance Level			
Gamma Statistics on Detected Data Only			
k hat (MLE)	1.265	k star (bias corrected MLE)	0.874
Theta hat (MLE)	2.326	Theta star (bias corrected MLE)	3.366
nu hat (MLE)	20.23	nu star (bias corrected)	13.98
MLE Mean (bias corrected)	2.941		
MLE Sd (bias corrected)	3.147	95% Percentile of Chisquare (2k)	5.492

TCE (continued) - Output Screen for All BTV Estimates (Left-Censored Data Set with NDs)

The following statistics are computed using Gamma ROS Statistics on Imputed Data					
Upper Limits using Wilson Hilferty (WH) and Hawkins Wixley (HW) Methods					
	WH	HW		WH	HW
95% Approx. Gamma UTL with 95% Coverage	19.62	27.19	95% Approx. Gamma UPL	9.793	11.66
95% Gamma USL	13.95	17.89			
The following statistics are computed using gamma distribution and KM estimates					
Upper Limits using Wilson Hilferty (WH) and Hawkins Wixley (HW) Methods					
k hat (KM)	0.702		nu hat (KM)	16.86	
	WH	HW		WH	HW
95% Approx. Gamma UTL with 95% Coverage	11.34	11.95	95% Approx. Gamma UPL	6.88	6.896
95% Gamma USL	8.836	9.063			
Lognormal GOF Test on Detected Observations Only					
Shapiro Wilk Test Statistic	0.865		Shapiro Wilk GOF Test		
5% Shapiro Wilk Critical Value	0.818		Detected Data appear Lognormal at 5% Significance Level		
Lilliefors Test Statistic	0.258		Lilliefors GOF Test		
5% Lilliefors Critical Value	0.313		Detected Data appear Lognormal at 5% Significance Level		
Detected Data appear Lognormal at 5% Significance Level					
Background Lognormal ROS Statistics Assuming Lognormal Distribution Using Imputed Non-Detects					
Mean in Original Scale	2.018		Mean in Log Scale	-0.214	
SD in Original Scale	2.838		SD in Log Scale	1.512	
95% UTL95% Coverage	50.54		95% BCA UTL95% Coverage	9.29	
95% Bootstrap (%) UTL95% Coverage	9.29		95% UPL (t)	13.63	
90% Percentile (z)	5.606		95% Percentile (z)	9.71	
99% Percentile (z)	27.2		95% USL	25.55	
Statistics using KM estimates on Logged Data and Assuming Lognormal Distribution					
KM Mean of Logged Data	0.294		95% KM UTL (Lognormal)95% Coverage	15.25	
KM SD of Logged Data	0.888		95% KM UPL (Lognormal)	7.06	
95% KM Percentile Lognormal (z)	5.784		95% KM USL (Lognormal)	10.21	
Nonparametric Uppper Limits for BTVs(no distinction made between detects and nondetects)					
Order of Statistic, r	12		95% UTL with95% Coverage	9.29	
Approximate f	0.632		Confidence Coefficient (CC) achieved by UTL	0.46	
95% UPL	9.29		95% USL	9.29	

Note: Even though the data set failed the Shapiro-Wilk test of normality, based upon Lilliefors test it was concluded that the data set follows a normal distribution. Therefore, instead of saying that the data set does not follow a normal distribution, ProUCL outputs that the data set follows an approximate normal distribution. In practice the two tests can lead to different conclusions, especially when the data set is of small size. In such instances, the user may want to select a distribution (if any) passing both of the GOF tests. It is also suggested that the user supplements test results with graphical displays to derive the final conclusion.

As noted, detected data follow a gamma as well as a lognormal distribution. The various upper limits using Gamma ROS and Lognormal ROS methods and Gamma and Lognormal distribution on KM estimates are summarized as follows.

Summary of Upper Limits Computed using Gamma and Lognormal Distribution of Detected Data
Sample Size = 12, No. of NDs = 4, % NDs = 33.33, Max Detect = 9.29

Upper Limits	Gamma Distribution		Lognormal Distribution	
	Result	Reference/ Method of Calculation	Result	Reference/ Method of Calculation
Mean (KM)	2.188	--	0.29	Logged
Mean (ROS)	1.964	--	2.018	--
UPL95 (ROS)	9.79	WH- ProUCL(ROS)	13.63	Helsel (2012), EPA (2009)-LROS
UTL95-95 (ROS)	19.62	WH- ProUCL(ROS)	50.54	Helsel (2012), EPA (2009)-LROS
UPL95 (KM)	6.88	WH - ProUCL (KM-Gamma)	7.06	KM-Lognormal EPA (2009)
UTL95-95 (KM)	11.34	WH - ProUCL (KM-Gamma)	15.25	KM- Lognormal EPA(2009)

Note: All computations have been performed using the ProUCL software. In the above table, methods proposed/described in the literature have been cited in the Reference Method of Calculation column. The statistics summarized above demonstrate the merits of using the gamma distribution based upper limits to estimate decision parameters (BTVs) of interest. These results summarized in the above tables suggest that the use of a gamma distribution cannot be dismissed just because it is easier to use a lognormal distribution to model skewed data sets as stated by some practitioners.

Chapter 11

Computing Upper Confidence Limits (UCLs) of Mean Based Upon Full-Uncensored Data Sets and Left-Censored Data Sets with Nondetects

Several parametric and nonparametric UCL methods for full-uncensored and left-censored data sets consisting of ND observations with multiple DLs are available in ProUCL 5.1. Methods such as the Kaplan-Meier (KM) and regression on order statistics (ROS) methods incorporated in ProUCL can handle multiple detection limits. For details regarding the goodness-of-fit tests and UCL computation methods available in ProUCL, consult the ProUCL Technical Guides, Singh, Singh, and Engelhardt (1997); Singh, Singh, and Iaci (2002); and Singh, Maichle, and Lee (2006).

In ProUCL 5.0/ProUCL 5.1, two choices are available for computing UCL statistics:

- <u>Full (w/o NDs):</u> Computes UCLs for full-uncensored data sets without any nondetects.

- <u>With NDs:</u> Computes UCLs for data sets consisting of ND observations with multiple DLs or reporting limits (RLs).

- For full data sets without NDs and also for data sets with NDs, the following options and choices are available to compute UCLs of the population mean.

    - The user specifies a confidence level; a number in the interval (0.5, 1), 0.5 inclusive. The default choice is 0.95.

    - The program computes several nonparametric UCLs using the CLT, adjusted CLT, Chebyshev inequality, jackknife, and bootstrap re-sampling methods.

    - For the bootstrap method, the user can select the number of bootstrap runs (re-samples). The default choice for the number of bootstrap runs is 2000.

    - The user is responsible for selecting an appropriate choice for the data distribution: normal, gamma, lognormal, or nonparametric. It is desirable that user determines data distribution using the Goodness-of-Fit test option prior to using the UCL option. The UCL output sheet also informs the user if data are normal, gamma, lognormal, or a non-discernible distribution. Program computes statistics depending on the user selection.

    - For data sets, which are not normal, one may try the gamma UCL next. The program will offer you advice if you chose the wrong UCL option.

    - For data sets, which are neither normal nor gamma, one may try the lognormal UCL. The program will offer you advice if you chose the wrong UCL option.

- Data sets that are not normal, gamma, or lognormal are classified as distribution-free nonparametric data sets. The user may use nonparametric UCL option for such data sets. The program will offer you advice if you chose the wrong UCL option.

- The program also provides the **All** option. By selecting this option, ProUCL outputs most of the relevant UCLs available in ProUCL. The program informs the user about the distribution of the underlying data set, and offers advice regarding the use of an appropriate UCL.

  For lognormal data sets, ProUCL can compute 90%, 95%, 97.5%, and 99% Land's statistic-based H-UCL of the mean. For all other methods, ProUCL can compute a UCL for any confidence coefficient (CC) in the interval (0.5, 1.0), 0.5 inclusive. If you have selected a distribution, then ProUCL will provide a recommended UCL method for 0.95, confidence level. Even though ProUCL can compute UCLs for any confidence coefficient level in the interval (0.5, 1.0), the recommendations are provided only for 95% UCL; as EPC term is estimated by a 95% UCL of the mean.

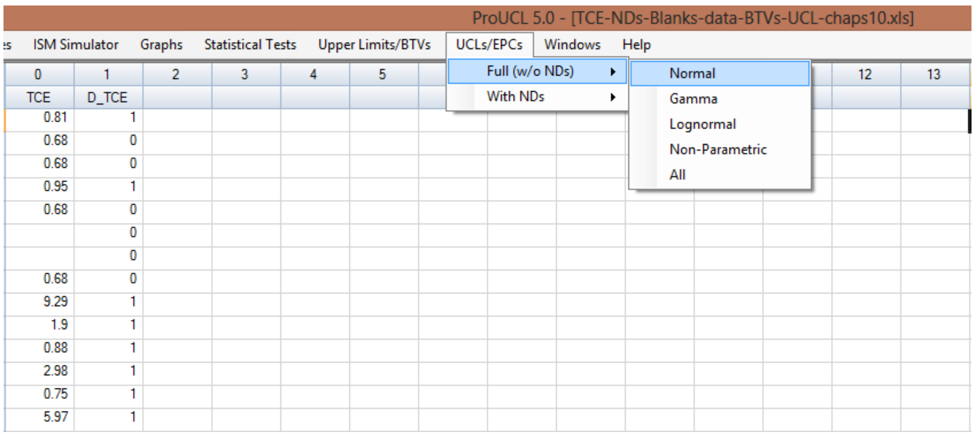
Notes: Like all other methods, it is recommended that the user identify a few low probability (coming from extreme tails) outlying observations that may be present in the data set. Outliers distort statistics of interest including summary statistics, data distributions, test statistics, UCLs and BTVs. Decisions based upon distorted statistics may be misleading and incorrect. The objective is to compute decision statistics based upon the majority of the data set representing the main dominant population. The project team should decide about the disposition (to include or not to include) of outliers before computing estimates of EPCs and BTVs. To determine the influence of outliers on UCLs and background statistics, the project team may want to compute statistics twice: once using the data set with outliers, and once using the data set without outliers.

Note on Computing Lower Confidence Limits (LCLs) of the Mean: In several environmental applications, one needs to compute a LCL of the population mean. At present, ProUCL does not directly compute LCLs of mean. It should be pointed out that for data sets with and without NDs, except for the bootstrap methods, gamma distribution (e.g., samples of sizes <50), and H-statistic based LCL of mean, the same critical value (e.g., normal z value, Chebyshev critical value, or t-critical value) are used to compute a LCL of mean as used in the computation of the UCL of mean. Specifically, to compute a LCL, the '+' sign used in the computation of the corresponding UCL needs to be replaced by the '-' sign in the equation used to compute that UCL (excluding gamma, lognormal H-statistic, and bootstrap methods). For specific details, the user may want to consult a statistician. For data sets *without nondetect* observations, the user may want to use the Scout 2008 software package (EPA 2009c) to directly compute the various parametric and nonparametric LCLs of mean.

11.1 UCLs for Full (w/o NDs) Data Sets

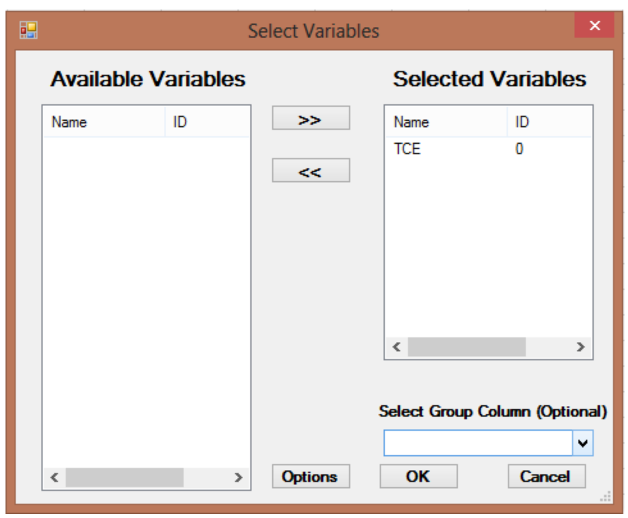
11.1.1 Normal Distribution (Full Data Sets without NDs)

1. Click **UCLs/EPCs ► Full (w/o NDs) ► Normal**

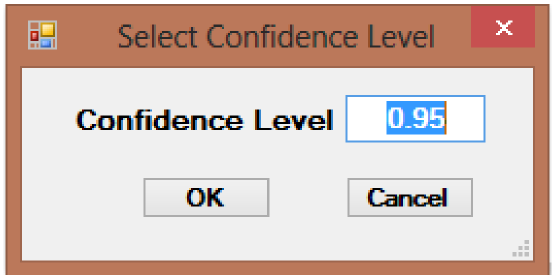


2. The **Select Variables** screen (Chapter 3) will appear.

- Select a variable(s) from the **Select Variables** screen.
- If needed, select a group variable by clicking the arrow below the **Select Group Column (Optional)** to obtain a drop-down list of available variables to select a group variable.



- When the **Option** button is clicked, the following window will be shown.



- Specify the **Confidence Level**; a number in the interval (0.5, 1), 0.5 inclusive. The default choice is **0.95**.
- Click on **OK** button to continue or on **Cancel** button to cancel the option.

* Click on **OK** to continue or on **Cancel** to cancel the UCL computation option.

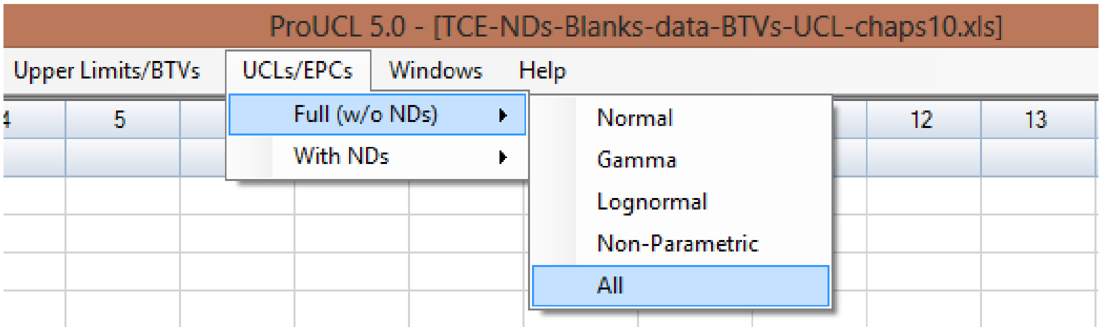
Example 11-1. Consider the data used in Example 1-1 collected from a Superfund site; vanadium concentrations follow a normal distribution. The normal distribution based 95% UCLs of mean are summarized in the following table.

Vanadium - Output Screen for Normal Distribution (Full Data w/o NDs)

Normal UCL Statistics for Uncensored Full Data Sets			
User Selected Options			
Date/Time of Computation	3/25/2013 3:53:05 PM		
From File	SuperFund.xls		
Full Precision	OFF		
Confidence Coefficient	95%		
Vanadium			
General Statistics			
Total Number of Observations	20	Number of Distinct Observations	17
		Number of Missing Observations	0
Minimum	7.2	Mean	17.34
Maximum	32	Median	16.5
SD	8.075	SD of logged Data	0.492
Coefficient of Variation	0.466	Skewness	0.429
Normal GOF Test			
Shapiro Wilk Test Statistic	0.925	**Shapiro Wilk GOF Test**	
5% Shapiro Wilk Critical Value	0.905	Data appear Normal at 5% Significance Level	
Lilliefors Test Statistic	0.146	**Lilliefors GOF Test**	
5% Lilliefors Critical Value	0.198	Data appear Normal at 5% Significance Level	
Data appear Normal at 5% Significance Level			
Assuming Normal Distribution			
95% Normal UCL		**95% UCLs (Adjusted for Skewness)**	
95% Student's-t UCL	20.46	95% Adjusted-CLT UCL (Chen-1995)	20.49
		95% Modified-t UCL (Johnson-1978)	20.49
Suggested UCL to Use			
95% Student's-t UCL	20.46		

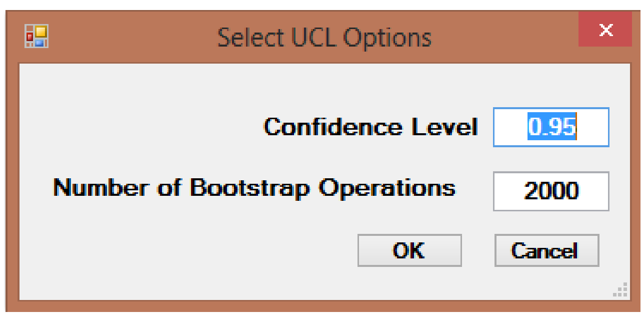
11.1.2 Gamma, Lognormal, Nonparametric, All Statistics Option (Full Data without NDs)

1. Click **UCLs/EPCs ► Full (w/o NDs) ► Gamma, Lognormal, Non-Parametric, or All**



2. The **Select Variables** screen (Chapter 3) will appear.

   - Select a variable(s) from the **Select Variables** screen.
   - If needed, select a group variable by clicking the arrow below the **Select Group Column (Optional)** to obtain a drop-down list of available variables, and select a proper group variable.
   - When the **Option** button is clicked, the following window will be shown.



     - Specify the **Confidence Level**; a number in the interval [0.5, 1), 0.5 inclusive.
     - Specify the **Number of Bootstrap Operations (runs)**. Default choice is **2000**.
     - Click on **OK** button to continue or on **Cance**l button to cancel the UCLs option.

   - Click on **OK** to continue or on **Cancel** to cancel the selected UCL computation option.

Example 11-2: This skewed data set of size n=25 with mean=44.09 was used in Chapter 2 of the Technical Guide. The data follows a lognormal and a gamma distribution. The data are: 0.3489, 0.8526, 2.5445, 2.5602, 3.3706, 4.8911, 5.0930, 5.6408, 7.0407, 14.1715, 15.2608, 17.6214, 18.7690, 23.6804, 25.0461, 31.7720, 60.7066, 67.0926, 72.6243, 78.8357, 80.0867, 113.0230, 117.0360, 164.3302, and 169.8303. UCLs based upon **Gamma**, **Lognormal**, **Non-parametric**, and **All** options are summarized in the following tables.

Output Screen for Gamma Distribution Based UCLs (Full [w/o NDs])

X			
General Statistics			
Total Number of Observations	25	Number of Distinct Observations	25
		Number of Missing Observations	0
Minimum	0.349	Mean	44.09
Maximum	169.8	Median	18.77
SD	51.34	SD of logged Data	1.68
Coefficient of Variation	1.164	Skewness	1.294
Gamma GOF Test			
A-D Test Statistic	0.374	**Anderson-Darling Gamma GOF Test**	
5% A-D Critical Value	0.794	Data appear Gamma Distributed at 5% Significance Level	
K-S Test Statistic	0.113	**Kolmogrov-Smirnoff Gamma GOF Test**	
5% K-S Critical Value	0.183	Data appear Gamma Distributed at 5% Significance Level	
Data appear Gamma Distributed at 5% Significance Level			
Gamma Statistics			
k hat (MLE)	0.643	k star (bias corrected MLE)	0.592
Theta hat (MLE)	68.58	Theta star (bias corrected MLE)	74.42
nu hat (MLE)	32.15	nu star (bias corrected)	29.62
MLE Mean (bias corrected)	44.09	MLE Sd (bias corrected)	57.28
		Approximate Chi Square Value (0.05)	18.2
Adjusted Level of Significance	0.0395	Adjusted Chi Square Value	17.59
Assuming Gamma Distribution			
95% Approximate Gamma UCL (use when n>=50)	71.77	95% Adjusted Gamma UCL (use when n<50)	74.27
Suggested UCL to Use			
95% Adjusted Gamma UCL	74.27		

Output Screen for Lognormal Distribution Based UCLs (Full [w/o NDs])

X			
General Statistics			
Total Number of Observations	25	Number of Distinct Observations	25
		Number of Missing Observations	0
Minimum	0.349	Mean	44.09
Maximum	169.8	Median	18.77
SD	51.34	Std. Error of Mean	10.27
Coefficient of Variation	1.164	Skewness	1.294
Lognormal GOF Test			
Shapiro Wilk Test Statistic	0.948	**Shapiro Wilk Lognormal GOF Test**	
5% Shapiro Wilk Critical Value	0.918	Data appear Lognormal at 5% Significance Level	
Lilliefors Test Statistic	0.135	**Lilliefors Lognormal GOF Test**	
5% Lilliefors Critical Value	0.177	Data appear Lognormal at 5% Significance Level	
Data appear Lognormal at 5% Significance Level			
Lognormal Statistics			
Minimum of Logged Data	-1.053	Mean of logged Data	2.835
Maximum of Logged Data	5.135	SD of logged Data	1.68
Assuming Lognormal Distribution			
95% H-UCL	229.2	90% Chebyshev (MVUE) UCL	140.6
95% Chebyshev (MVUE) UCL	176.3	97.5% Chebyshev (MVUE) UCL	225.8
99% Chebyshev (MVUE) UCL	323		
Suggested UCL to Use			
Data appear Gamma, May want to try Gamma_Distribution			

Output Screen for Nonparametric UCLs (Full [w/o NDs])

Nonparametric Distribution Free UCLs			
95% CLT UCL	60.98	95% Jackknife UCL	61.66
95% Standard Bootstrap UCL	60.44	95% Bootstrap-t UCL	65
95% Hall's Bootstrap UCL	62.14	95% Percentile Bootstrap UCL	61.42
95% BCA Bootstrap UCL	63.63		
90% Chebyshev(Mean, Sd) UCL	74.89	95% Chebyshev(Mean, Sd) UCL	88.85
97.5% Chebyshev(Mean, Sd) UCL	108.2	99% Chebyshev(Mean, Sd) UCL	146.3
Suggested UCL to Use			
Data appear Gamma, May want to try Gamma_Distribution			

Output Screen for All Statistics Option (Full [w/o NDs])

X			
General Statistics			
Total Number of Observations	25	Number of Distinct Observations	25
		Number of Missing Observations	0
Minimum	0.349	Mean	44.09
Maximum	169.8	Median	18.77
SD	51.34	Std. Error of Mean	10.27
Coefficient of Variation	1.164	Skewness	1.294
Normal GOF Test			
Shapiro Wilk Test Statistic	0.799	**Shapiro Wilk GOF Test**	
5% Shapiro Wilk Critical Value	0.918	Data Not Normal at 5% Significance Level	
Lilliefors Test Statistic	0.245	**Lilliefors GOF Test**	
5% Lilliefors Critical Value	0.177	Data Not Normal at 5% Significance Level	
Data Not Normal at 5% Significance Level			
Assuming Normal Distribution			
95% Normal UCL		**95% UCLs (Adjusted for Skewness)**	
95% Student's-t UCL	61.66	95% Adjusted-CLT UCL (Chen-1995)	63.82
		95% Modified-t UCL (Johnson-1978)	62.1
Gamma GOF Test			
A-D Test Statistic	0.374	**Anderson-Darling Gamma GOF Test**	
5% A-D Critical Value	0.794	Detected data appear Gamma Distributed at 5% Significance Level	
K-S Test Statistic	0.113	**Kolmogrov-Smirnoff Gamma GOF Test**	
5% K-S Critical Value	0.183	Detected data appear Gamma Distributed at 5% Significance Level	
Detected data appear Gamma Distributed at 5% Significance Level			

Continued: Output Screen for All Statistics Option (Full [w/o NDs])

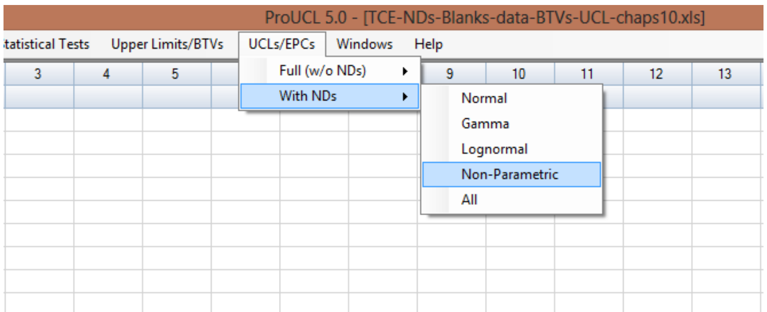
Gamma Statistics			
k hat (MLE)	0.643	k star (bias corrected MLE)	0.592
Theta hat (MLE)	68.58	Theta star (bias corrected MLE)	74.42
nu hat (MLE)	32.15	nu star (bias corrected)	29.62
MLE Mean (bias corrected)	44.09	MLE Sd (bias corrected)	57.28
		Approximate Chi Square Value (0.05)	18.2
Adjusted Level of Significance	0.0395	Adjusted Chi Square Value	17.59
Assuming Gamma Distribution			
95% Approximate Gamma UCL (use when n>=50)	71.77	95% Adjusted Gamma UCL (use when n<50)	74.27
Lognormal GOF Test			
Shapiro Wilk Test Statistic	0.948	**Shapiro Wilk Lognormal GOF Test**	
5% Shapiro Wilk Critical Value	0.918	Data appear Lognormal at 5% Significance Level	
Lilliefors Test Statistic	0.135	**Lilliefors Lognormal GOF Test**	
5% Lilliefors Critical Value	0.177	Data appear Lognormal at 5% Significance Level	
Data appear Lognormal at 5% Significance Level			
Lognormal Statistics			
Minimum of Logged Data	-1.053	Mean of logged Data	2.835
Maximum of Logged Data	5.135	SD of logged Data	1.68
Assuming Lognormal Distribution			
95% H-UCL	229.2	90% Chebyshev (MVUE) UCL	140.6
95% Chebyshev (MVUE) UCL	176.3	97.5% Chebyshev (MVUE) UCL	225.8
99% Chebyshev (MVUE) UCL	323		
Nonparametric Distribution Free UCL Statistics			
Data appear to follow a Discernible Distribution at 5% Significance Level			
Nonparametric Distribution Free UCLs			
95% CLT UCL	60.98	95% Jackknife UCL	61.66
95% Standard Bootstrap UCL	60.45	95% Bootstrap-t UCL	65.83
95% Hall's Bootstrap UCL	63.51	95% Percentile Bootstrap UCL	61.84
95% BCA Bootstrap UCL	64.96		
90% Chebyshev(Mean, Sd) UCL	74.89	95% Chebyshev(Mean, Sd) UCL	88.85
97.5% Chebyshev(Mean, Sd) UCL	108.2	99% Chebyshev(Mean, Sd) UCL	146.3
Suggested UCL to Use			
95% Adjusted Gamma UCL	74.27		

Notes: Once again, the statistics summarized above demonstrate the merits of using the gamma distribution based UCL of mean to estimate EPCs. The use of a lognormal distribution tends to yield unrealistic UCLs without practical merit (e.g., Lognormal UCL = 229.2 and the maximum = 169.8 in the above example). The results summarized in the above tables suggest that the use of a gamma distribution (when a data set follows a gamma distribution) cannot be dismissed just because it is easier (Helsel and Gilroy 2012) to use a lognormal distribution to model skewed data sets.

Number of valid samples represents the total number of samples minus (-) the missing values (if any). The number of unique or distinct samples simply represents number of distinct observations. The information about the number of distinct values is useful when using bootstrap methods. Specifically, it is not desirable to use bootstrap methods on data sets with only a few distinct values.

11.2 UCL for Left-Censored Data Sets with NDs

1. Click **UCLs/EPCs ► With NDs**



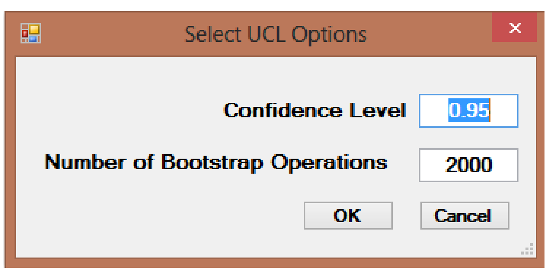
2. Choose the **Normal, Gamma, Lognormal, Non-Parametric,** or **All** option.

3. The **Select Variables** screen (Chapter 3) will appear.

   - Select a variable(s) from the **Select Variables** screen.

   - If needed, select a group variable by clicking the arrow below the **Select Group Column (Optional)** to obtain a drop-down list of available variables, and select a proper group variable. The selection of this option will compute the relevant statistics separately for each group that may be present in the data set.

   - When the **Option** button is clicked, the following window will be shown.



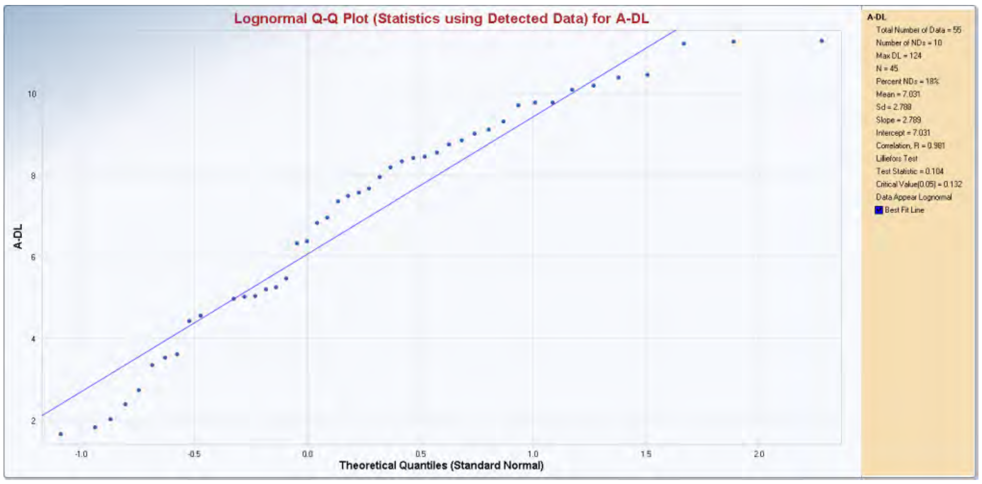
     - Specify the **Confidence Level**; a number in the interval (0.5, 1), 0.5 inclusive. The default choice is **0.95**.

     - Specify the **Number of Bootstrap Operations (runs)**. Default choice is **2000**.

     - Click on **OK** button to continue or on **Cancel** button to cancel the UCLs option.

   - Click on **OK** to continue or on **Cancel** to cancel the selected UCL computation option.

Example 11-3. This real data set of size n=55 with 18.8% NDs (=10) is also used in Chapters 4 and 5 of the ProUCL Technical Guide. The minimum detected value is 5.2 and the largest detected value is 79000, *sd* of detected logged data is 2.79 suggesting that the data set is highly skewed. The detected data follow a gamma as well as a lognormal distribution. It is noted that GROS data set with imputed values follows a gamma distribution and LROS data set with imputed values follows a lognormal distribution (results not included). The lognormal Q-Q plot based upon detected data is shown in the following figure. The various UCL output sheets: normal, nonparametric, gamma, and lognormal generated by ProUCL are summarized in tables following the lognormal Q-Q plot on detected data. The main results have been high-lighted in the output screen provided after the lognormal GOF Q-Q plot.



Output Screen for UCLs based upon Normal, Lognormal, and Gamma Distributions (of Detects)

A-DL			
General Statistics			
Total Number of Observations	55	Number of Distinct Observations	53
Number of Detects	45	Number of Non-Detects	10
Number of Distinct Detects	45	Number of Distinct Non-Detects	8
Minimum Detect	5.2	Minimum Non-Detect	3.8
Maximum Detect	79000	Maximum Non-Detect	124
Variance Detects	3.954E+8	Percent Non-Detects	18.18%
Mean Detects	10556	SD Detects	19886
Median Detects	1940	CV Detects	1.884
Skewness Detects	2.632	Kurtosis Detects	6.496
Mean of Logged Detects	7.031	SD of Logged Detects	2.788
Normal GOF Test on Detects Only			
Shapiro Wilk Test Statistic	0.575	**Shapiro Wilk GOF Test**	
5% Shapiro Wilk Critical Value	0.945	Detected Data Not Normal at 5% Significance Level	
Lilliefors Test Statistic	0.298	**Lilliefors GOF Test**	
5% Lilliefors Critical Value	0.132	Detected Data Not Normal at 5% Significance Level	
Detected Data Not Normal at 5% Significance Level			
Kaplan-Meier (KM) Statistics using Normal Critical Values and other Nonparametric UCLs			
Mean	8638	Standard Error of Mean	2488
SD	18246	95% KM (BCA) UCL	13562
95% KM (t) UCL	12802	95% KM (Percentile Bootstrap) UCL	13040
95% KM (z) UCL	12731	95% KM Bootstrap t UCL	15221
90% KM Chebyshev UCL	16102	95% KM Chebyshev UCL	19483
97.5% KM Chebyshev UCL	24176	99% KM Chebyshev UCL	33394

Continued: Output Screen for UCLs based upon Normal, Lognormal, and Gamma Distributions (of Detects)

Gamma GOF Tests on Detected Observations Only			
A-D Test Statistic	0.591	**Anderson-Darling GOF Test**	
5% A-D Critical Value	0.86	Detected data appear Gamma Distributed at 5% Significance Level	
K-S Test Statistic	0.115	**Kolmogrov-Smirnoff GOF**	
5% K-S Critical Value	0.143	Detected data appear Gamma Distributed at 5% Significance Level	
Detected data appear Gamma Distributed at 5% Significance Level			
Gamma Statistics on Detected Data Only			
k hat (MLE)	0.307	k star (bias corrected MLE)	0.302
Theta hat (MLE)	34333	Theta star (bias corrected MLE)	34980
nu hat (MLE)	27.67	nu star (bias corrected)	27.16
MLE Mean (bias corrected)	10556	MLE Sd (bias corrected)	19216
Gamma Kaplan-Meier (KM) Statistics			
k hat (KM)	0.224	nu hat (KM)	24.66
Approximate Chi Square Value (24.66, α)	14.35	Adjusted Chi Square Value (24.66, β)	14.14
95% Gamma Approximate KM-UCL (use when n>=50)	14844	95% Gamma Adjusted KM-UCL (use when n<50)	15066
GROS Statistics using imputed NDs			
Minimum	0.01	Mean	8637
Maximum	79000	Median	588
SD	18415	CV	2.132
k hat (MLE)	0.18	k star (bias corrected MLE)	0.183
Theta hat (MLE)	47915	Theta star (bias corrected MLE)	47314
nu hat (MLE)	19.83	nu star (bias corrected)	20.08
MLE Mean (bias corrected)	8637	MLE Sd (bias corrected)	20215
		Adjusted Level of Significance (β)	0.0456
Approximate Chi Square Value (20.08, α)	10.91	Adjusted Chi Square Value (20.08, β)	10.73
95% Gamma Approximate UCL (use when n>=50)	15896	95% Gamma Adjusted UCL (use when n<50)	16167
Lognormal GOF Test on Detected Observations Only			
Shapiro Wilk Test Statistic	0.939	**Shapiro Wilk GOF Test**	
5% Shapiro Wilk Critical Value	0.945	Detected Data Not Lognormal at 5% Significance Level	
Lilliefors Test Statistic	0.104	**Lilliefors GOF Test**	
5% Lilliefors Critical Value	0.132	Detected Data appear Lognormal at 5% Significance Level	
Detected Data appear Approximate Lognormal at 5% Significance Level			
Lognormal ROS Statistics Using Imputed Non-Detects			
Mean in Original Scale	8638	Mean in Log Scale	5.983
SD in Original Scale	18414	SD in Log Scale	3.391
95% t UCL (assumes normality of ROS data)	12793	95% Percentile Bootstrap UCL	13090
95% BCA Bootstrap UCL	14069	95% Bootstrap t UCL	15524
95% H-UCL (Log ROS)	1855231		
UCLs using Lognormal Distribution and KM Estimates when Detected data are Lognormally Distributed			
KM Mean (logged)	6.03	95% H-UCL (KM -Log)	1173988
KM SD (logged)	3.286	95% Critical H Value (KM-Log)	5.7
KM Standard Error of Mean (logged)	0.449		
Suggested UCL to Use			
95% KM (Chebyshev) UCL	19483	95% GROS Approximate Gamma UCL	15896
95% Approximate Gamma KM-UCL	14844		

Detected data follow a gamma as well as a lognormal distribution. The various upper limits using Gamma ROS and Lognormal ROS methods and Gamma and Lognormal distribution on KM estimates are summarized in the following table.

Upper Confidence Limits Computed using Gamma and Lognormal Distributions of Detected Data
Sample Size = 55, No. of NDs=10, % NDs = 18.18%

	Gamma Distribution		Lognormal Distribution	
Upper Limits	**Result**	**Reference/ Method of Calculation**	**Result**	**Reference/ Method of Calculation**
Min (detects)	5.2	--	1.65	Logged
Max (detects)	79000	--	11.277	Logged
Mean (KM)	8638	--	6.3	Logged
Mean (ROS)	8637	--	8638	--
UCL95 (ROS)	15896	ProUCL 5.0 -GROS	14863	bootstrap-t on LROS, ProUCL 5.0
			12918	percentile bootstrap on LROS, Helsel(2012)
UCL (KM)	14844	ProUCL 5.0 - KM-Gamma	1173988	H-UCL, KM mean and *sd* on logged data, EPA (2009)

- All computations have been performed using the ProUCL software. In the above table, methods proposed/described in the literature have been cited in the Reference Method of Calculation column. The results summarized in the above table re-iterate that the use of a gamma distribution cannot be dismissed just because it is easier to use a lognormal distribution to model skewed data sets. These results also demonstrate that for skewed data sets, one should use bootstrap methods which adjust for data skewness (e.g., bootstrap- t method) rather than using percentile bootstrap method.

Chapter 12

Sample Sizes Based Upon User Specified Data Quality Objectives (DQOs) and Power Assessment

One of the most frequent problems in the application of statistical theory to practical applications, including environmental projects, is to determine the minimum number of samples needed for sampling of reference/background areas and survey units (e.g., potentially impacted site areas, areas of concern, decision units) to make cost-effective and defensible decisions about the population parameters based upon the sampled discrete data. The sample size determination formulae for estimation of the population mean (or some other parameters) depend upon certain decision parameters including the confidence coefficient, $(1\text{-}\alpha)$ and the specified error margin (difference), Δ from the unknown true population mean, μ. Similarly, for hypotheses testing approaches, sample size determination formulae depend upon pre-specified values of the decision parameters selected while describing the data quality objectives (DQOs) associated with an environmental project. The decision parameters associated with hypotheses testing approaches include Type I (false positive error rate, α) and Type II (false negative error rate, β=1-power) error rates; and the allowable width, Δ of the gray region. For values of the parameter of interest (e.g., mean, proportion) lying in the gray region, the consequences of committing the two types of errors described above are not significant from both human health and cost-effectiveness point of view.

Note: Initially, the **Sample Sizes** module was incorporated in ProUCL 4.0/ProUCL 4.1. Not many changes have been made in ProUCL 5.0/ProUCL 5.1 except those described below. Therefore, many screenshots generated using an earlier 2010 version of ProUCL have been used in the examples described in this chapter.

Both parametric (assuming normality) and nonparametric (distribution free) sample size determination formulae as described in guidance documents (MARSSIM 2000, EPA 2002c and 2006a) have been incorporated in the ProUCL software. Specifically, the **DQOs Based Sample Sizes** module of ProUCL can be used to determine sample sizes to estimate the mean, perform parametric and nonparametric single-sample and two-sample hypothesis tests, and apply acceptance sampling approaches to address project needs of the various CERCLA and RCRA site projects. The details can be found in Chapter 8 of the ProUCL Technical Guide and in EPA guidance documents (EPA 2006a, 2006b).

New in ProUCL 5.0/ProUCL 5.1: The Sample size module in ProUCL 5.0/ProUCL 5.1 can be used at two different stages of a project. Most of the sample size formulae require some estimate of the population standard deviation (variability). Depending upon the project stage, a standard deviation: 1) represents a preliminary estimate of the population (e.g., study area) variability needed to compute the minimum sample size during the planning and design stage; or 2) represents the sample standard deviation computed using the data collected without considering DQOs process which is used to assess the power of the test based upon the collected data. During the power assessment stage, if the computed sample size is larger than the size of already collected data set, it can be inferred that the size of the collected data set is not large enough to achieve the desired power. The formulae to compute the sample sizes during the planning stage and after performing a statistical test are the same except that the estimates of standard deviations are computed/estimated differently.

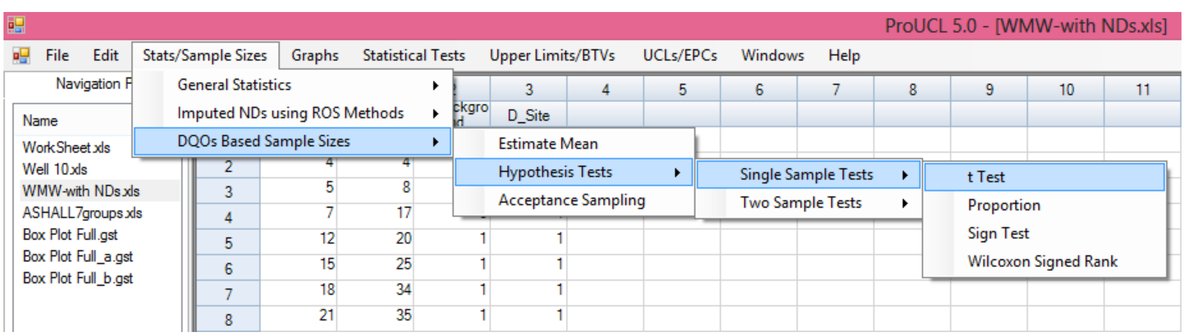
Planning stage before collecting data: Sample size formulae are commonly used during the planning stage of a project to determine the minimum sample sizes needed to address project objectives (estimation, hypothesis testing) with specified values of the decision parameters (e.g., Type I and II errors, width of gray region). During the planning stage, since the data are not collected *a priori*, a preliminary rough estimate of the population standard deviation (to be expected in sampled data) is obtained from other similar sites, pilot studies, or expert opinions. An estimate of the expected standard deviation along with the specified values of the other decision parameters are used to compute the minimum sample sizes needed to address the project objectives during the sampling planning stage; the project team is expected to collect the number of samples thus obtained. The detailed discussion of the sample size determination approaches during the planning stage can be found in MARSSIM 2000 and U.S. EPA 2006a.

<u>Power assessment stage after performing a statistical method:</u> Often, in practice, environmental samples/data sets are collected without taking the DQOs process into consideration. Under this scenario, the project team performs statistical tests on the available already collected data set. However, once a statistical test (e.g., WMW test) has been performed, the project team can assess the power associated with the test in retrospect. That is for specified DQOs and decision errors (Type I error and power of the test [=1-Type II error]), using the sample standard deviation computed based upon the already collected data, the minimum sample size needed to perform the test for specified values of the decision parameters is computed.

- If the computed sample size obtained using the sample variance is less than the size of the already collected data set used to perform the test, it may be determined that the power of the test has been achieved. However, if the sample size of the collected data is less than the minimum sample size computed in retrospect, the user may want to collect additional samples to assure that the test achieves the desired power.

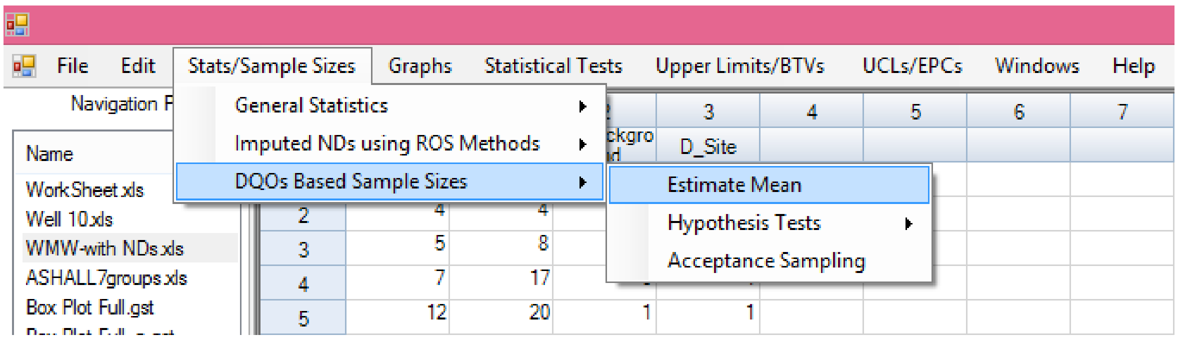
- It should be pointed out that there could be differences in the sample sizes computed in two different stages due to the differences in the values of the estimated variability. Specifically, the preliminary estimate of the variance computed using information from similar sites could be significantly different from the variance computed using the available data already collected from the study area under investigation which will yield different values of the sample size.

Sample size determination methods in ProUCL can be used for both stages. The only difference will be in the input value of the standard deviation/variance. It is user's responsibility to input a correct value for the standard deviation during the two stages.

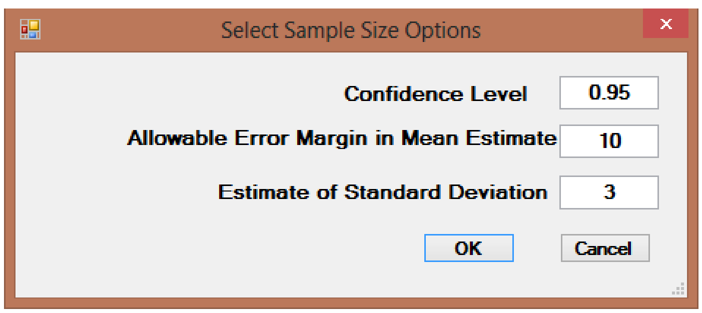


12.1 Estimation of Mean

1. Click **Stats/Sample Sizes► DQOs Based Sample Sizes ► Estimate Mean**

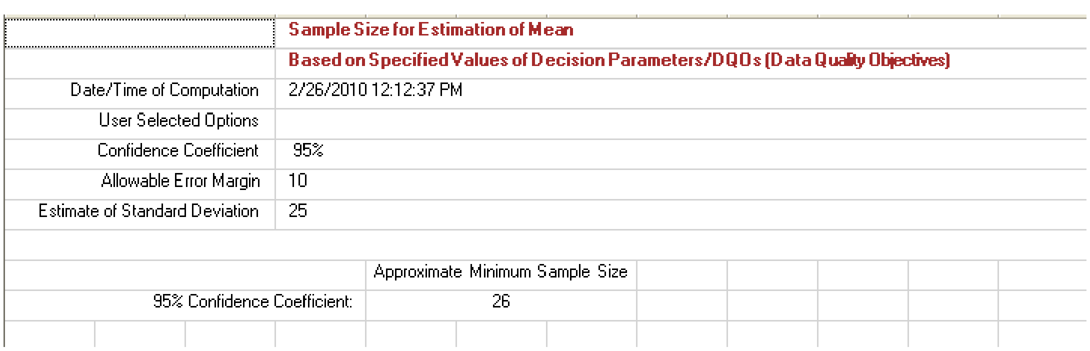


2. The following options window is shown.



- Specify the **Confidence Coefficient**. Default is **0.95**.
- Specify the **Estimate of standard deviation**. Default is **3.**
- Specify the **Allowable Error Margin in Mean Estimate**. Default is **10**.
- Click on **OK** button to continue or on **Cancel** button to cancel the options.

Output Screen for Sample sizes for Estimation of Mean (CC = 95%, *sd* = 25, Error Margin = 10)

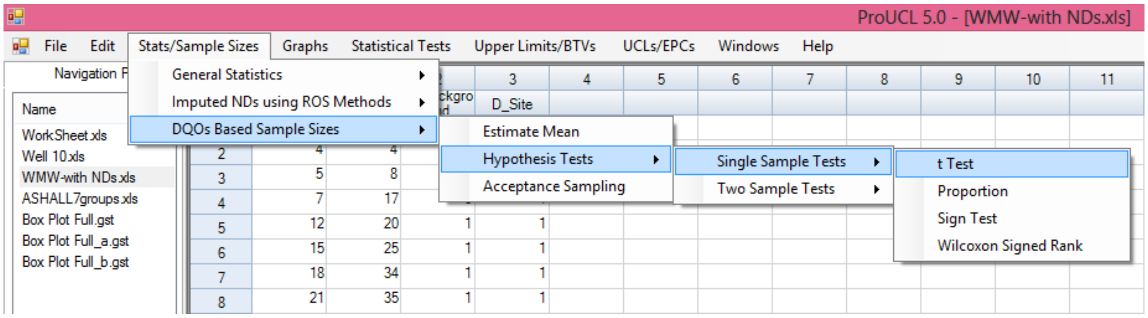


	Sample Size for Estimation of Mean	
	Based on Specified Values of Decision Parameters/DQOs (Data Quality Objectives)	
Date/Time of Computation	2/26/2010 12:12:37 PM	
User Selected Options		
Confidence Coefficient	95%	
Allowable Error Margin	10	
Estimate of Standard Deviation	25	
		Approximate Minimum Sample Size
95% Confidence Coefficient:		26

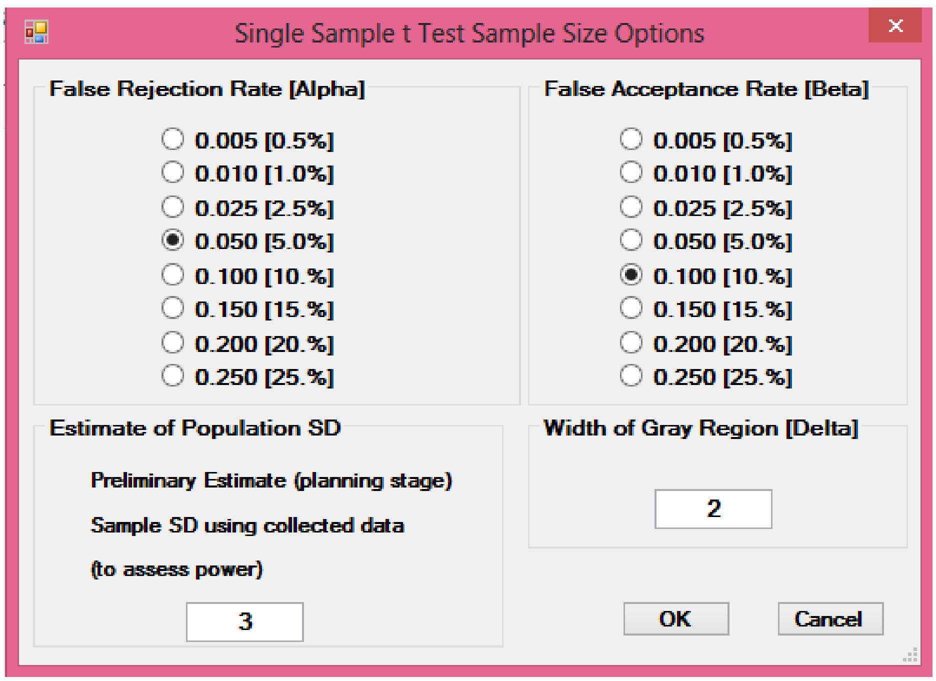
12.2 Sample Sizes for Single-Sample Hypothesis Tests

12.2.1 Sample Size for Single-Sample t-Test

1. Click **DQOs Based Sample Sizes ► Hypothesis Tests► Single Sample Tests► t Test**



- The following options window is shown.



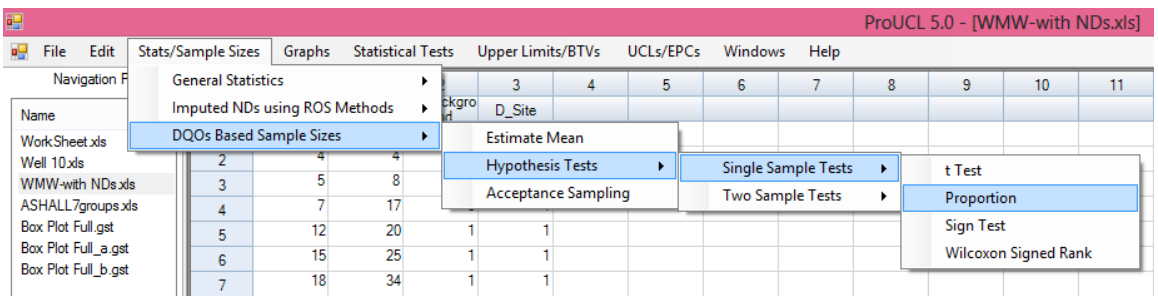
- Specify the **False Rejection Rate (Alpha, α)**. Default is **0.05**.
- Specify the **False Acceptance Rate (Beta, β)**. Default is **0.1**.
- Specify the **Estimate of standard deviation**. Default is **3.**
- Specify the **Width of the Gray Region (Delta, Δ)**. Default is **2**.
- Click on **OK** button to continue or on **Cancel** button to cancel the options.

Output Screen for Sample Sizes for Single-Sample t-Test ($\alpha = 0.05$, $\beta = 0.2$, $sd = 10.41$, $\Delta = 10$) Example from EPA 2006a (page 49)

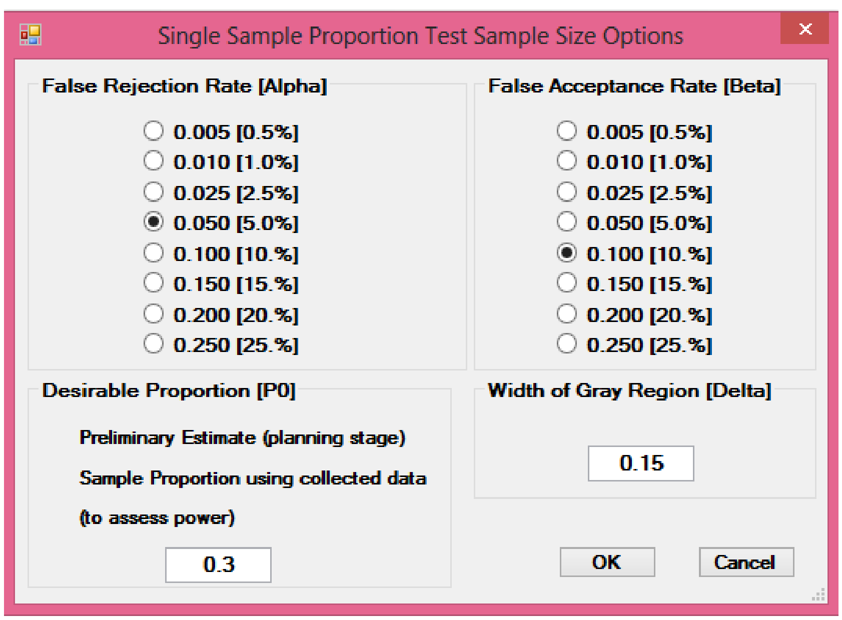
	Sample Sizes for Single Sample t Test					
	Based on Specified Values of Decision Parameters/DQOs (Data Quality Objectives)					
Date/Time of Computation	2/26/2010 12:41:58 PM					
User Selected Options						
False Rejection Rate [Alpha]	0.05					
False Acceptance Rate [Beta]	0.2					
Width of Gray Region [Delta]	10					
Estimate of Standard Deviation	10.41					
	Approximate Minimum Sample Size					
Single Sided Alternative Hypothesis:	9					
Two Sided Alternative Hypothesis:	11					

12.2.2 Sample Size for Single-Sample Proportion Test

1. Click **DQOs Based Sample Sizes ► Hypothesis Tests► Single Sample Tests► Proportion**



2. The following options window is shown.



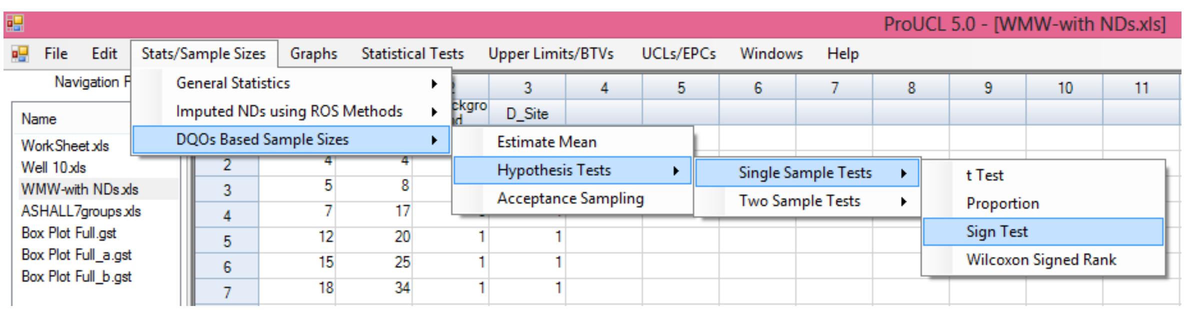
- Specify the **False Rejection Rate (Alpha, *α*)**. Default is **0.05**.
- Specify the **False Acceptance Rate (Beta, *β*)**. Default is **0.1**.
- Specify the **Desirable Proportion (P0)**. Default is **0.3.**
- Specify the **Width of the Gray Region (Delta, *Δ*)**. Default is **0.15**.
- Click on **OK** button to continue or on **Cancel** button to cancel the options.

Output Screen for Sample Size for Single-Sample Proportion Test (α = 0.05, β = 0.2, $P0$ = 0.2, Δ = 0.05) Example from EPA 2006a (page 59)

	Sample Sizes for Single Sample Proportion Test
	Based on Specified Values of Decision Parameters/DQOs (Data Quality Objectives)
Date/Time of Computation	2/26/2010 12:50:52 PM
User Selected Options	
False Rejection Rate [Alpha]	0.05
False Acceptance Rate [Beta]	0.2
Width of Gray Region [Delta]	0.05
Proportion/Action Level [P0]	0.2
	Approximate Minimum Sample Size
Right Sided Alternative Hypothesis:	419
Left Sided Alternative Hypothesis:	368
Two Sided Alternative Hypothesis:	max(471, 528)

12.2.3 Sample Size for Single-Sample Sign Test

1. Click **DQOs Based Sample Sizes ► Hypothesis Tests► Single Sample Tests► Sign Test**



2. The following options window is shown.

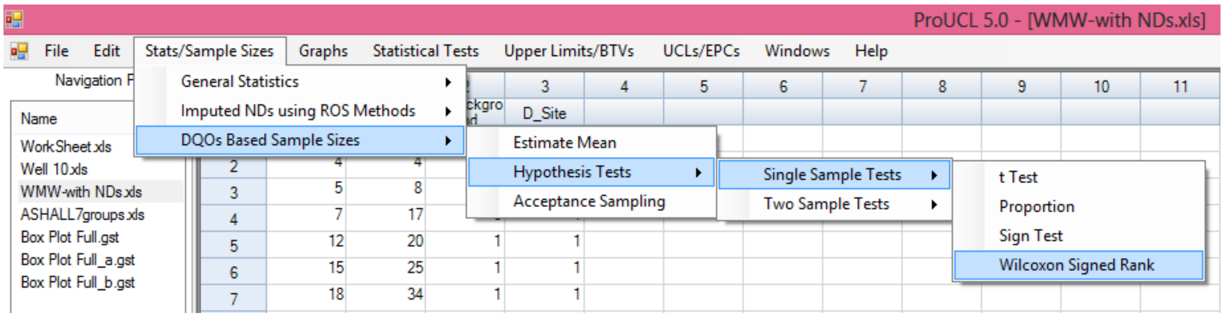
- Specify the **False Rejection Rate (Alpha, α)**. Default is **0.05**.
- Specify the **False Acceptance Rate (Beta, β)**. Default is **0.1**.
- Specify the **Estimate of standard deviation**. Default is **3**
- Specify the **Width of the Gray Region (Delta, Δ)**. Default is **2**.
- Click on **OK** button to continue or on **Cancel** button to cancel the options.

Output Screen for Sample Sizes for Single-Sample Sign Test (Default Options)

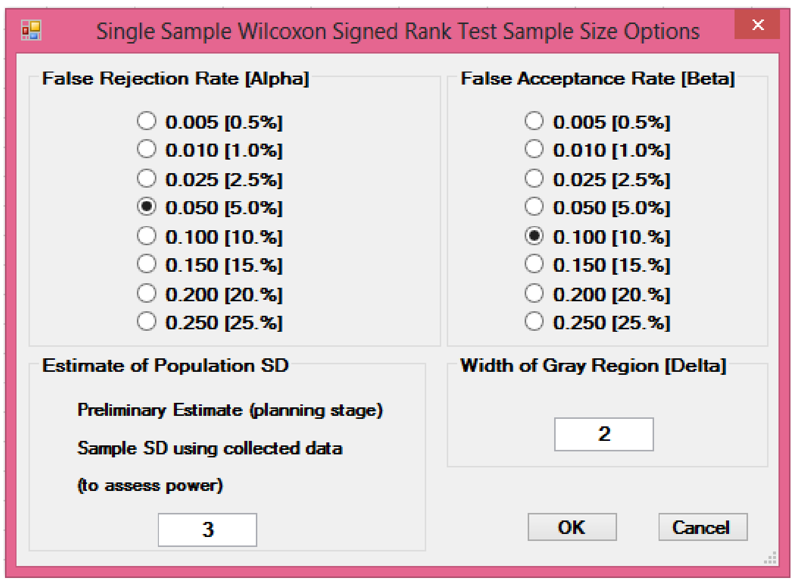
	Sample Sizes for Single Sample Sign Test					
	Based on Specified Values of Decision Parameters/DQOs (Data Quality Objectives)					
Date/Time of Computation	2/26/2010 12:15:27 PM					
User Selected Options						
False Rejection Rate [Alpha]	0.05					
False Acceptance Rate [Beta]	0.1					
Width of Gray Region [Delta]	2					
Estimate of Standard Deviation	3					
	Approximate Minimum Sample Size					
Single Sided Alternative Hypothesis:	35					
Two Sided Alternative Hypothesis:	43					

12.2.4 Sample Size for Single-Sample Wilcoxon Signed Rank Test

1. Click **DQOs Based Sample Sizes ► Hypothesis Tests► Single Sample Tests► Wilcoxon Signed Rank**



2. The following options window is shown.



- Specify the **False Rejection Rate (Alpha, α)**. Default is **0.05**.
- Specify the **False Acceptance Rate (Beta, β)**. Default is **0.1**.
- Specify the **Estimate of standard deviation of WSR Test Statistic**. Default is **3**
- Specify the **Width of the Gray Region (Delta, Δ)**. Default is **2**.
- Click on **OK** button to continue or on **Cancel** button to cancel the options.

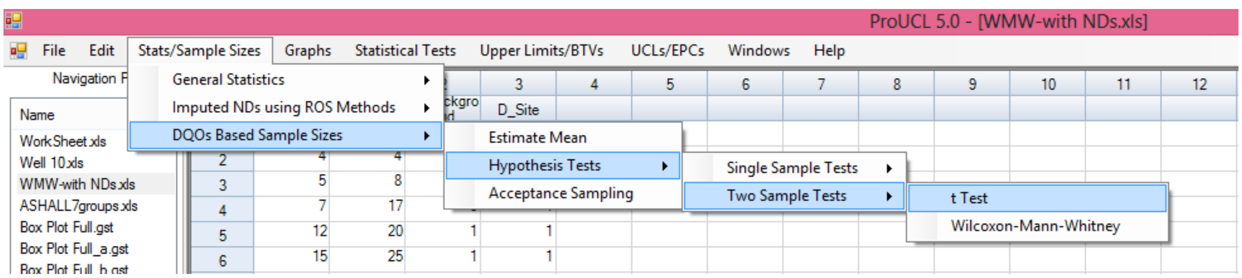
Output Screen for Sample Sizes for Single-Sample WSR Test (α = 0.1, β = 0.2, *sd* = 130, Δ = 100) Example from EPA 2006a (page 65)

	Sample Sizes for Single Sample Wilcoxon Signed Rank Test					
	Based on Specified Values of Decision Parameters/DQOs (Data Quality Objectives)					
Date/Time of Computation	2/26/2010 1:13:58 PM					
User Selected Options						
False Rejection Rate [Alpha]	0.1					
False Acceptance Rate [Beta]	0.2					
Width of Gray Region [Delta]	100					
Estimate of Standard Deviation	130					
	Approximate Minimum Sample Size					
Single Sided Alternative Hypothesis:	10					
Two Sided Alternative Hypothesis:	14					

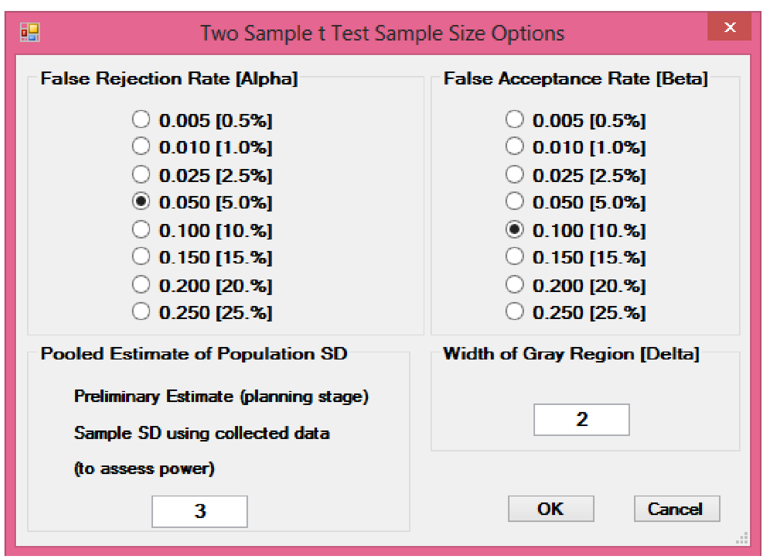
12.3 Sample Sizes for Two-Sample Hypothesis Tests

12.3.1 Sample Size for Two-Sample t-Test

1. Click **DQOs Based Sample Sizes ► Hypothesis Tests► Two Sample Tests► t Test**



The following options window is shown.



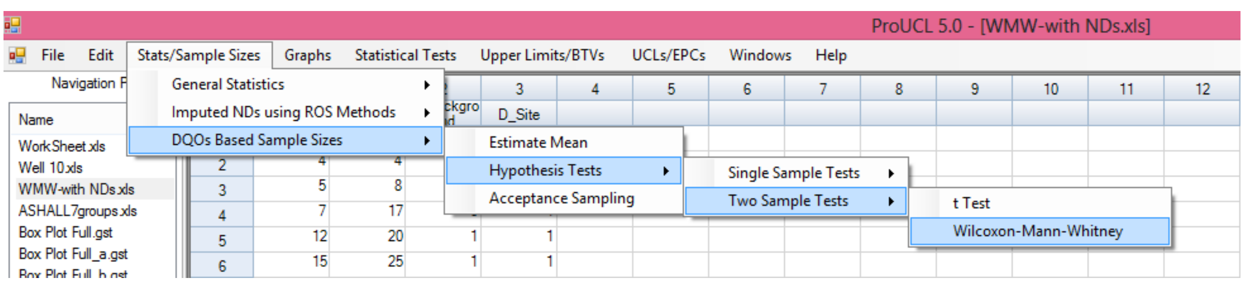
- Specify the **False Rejection Rate (Alpha, α)**. Default is **0.05**.
- Specify the **False Acceptance Rate (Beta, β)**. Default is **0.1**.
- Specify the **Estimate of standard deviation**. Default is **3**
- Specify the **Width of the Gray Region (Delta, Δ)**. Default is **2**.
- Click on **OK** button to continue or on **Cancel** button to cancel the options.

Output Screen for Sample Sizes for Two-Sample t-Test (α = 0.05, β = 0.2, s_p = 1.467, Δ = 2.5) Example from EPA 2006a (page 68)

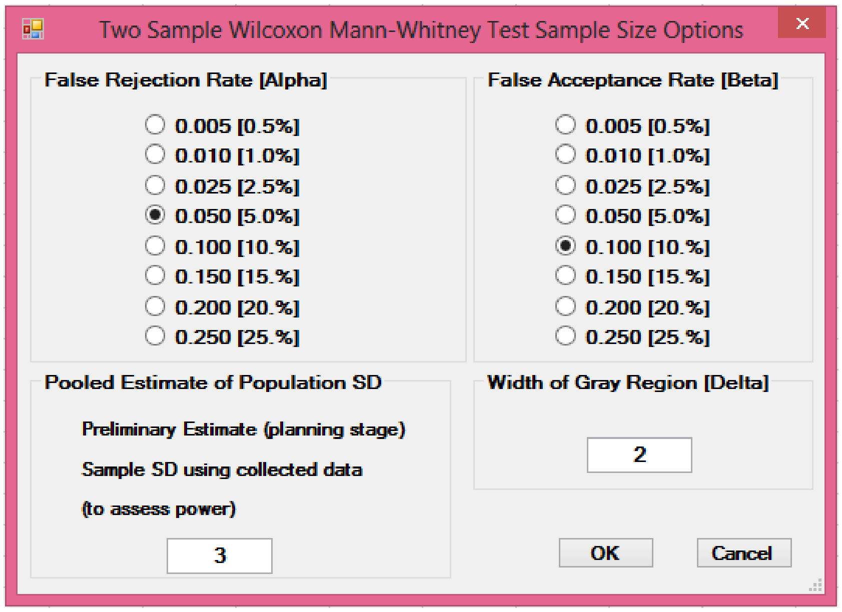
	Sample Sizes for Two Sample t Test					
	Based on Specified Values of Decision Parameters/DQOs (Data Quality Objectives)					
Date/Time of Computation	2/26/2010 1:17:57 PM					
User Selected Options						
False Rejection Rate [Alpha]	0.05					
False Acceptance Rate [Beta]	0.2					
Width of Gray Region [Delta]	2.5					
Estimate of Pooled SD	1.467					
	Approximate Minimum Sample Size					
Single Sided Alternative Hypothesis:	5					
Two Sided Alternative Hypothesis:	7					

12.3.2 Sample Size for Two-Sample Wilcoxon Mann-Whitney Test

1. Click **DQOs Based Sample Sizes ► Hypothesis Tests► Two Sample Tests► Wilcoxon-Mann-Whitney**



2. The following options window is shown.



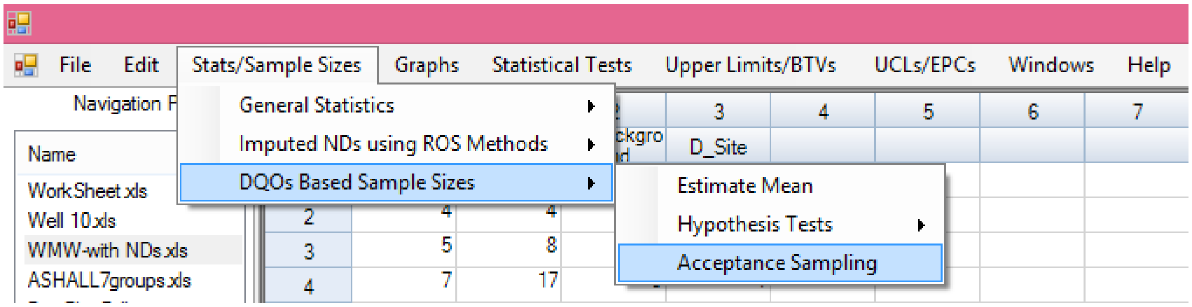
- Specify the **False Rejection Rate (Alpha, α)**. Default is **0.05**.
- Specify the **False Acceptance Rate (Beta, β)**. Default is **0.1**.
- Specify the **Estimate of standard deviation of WMW Test Statistic**. Default is **3**
- Specify the **Width of the Gray Region (Delta, Δ)**. Default is **2**.
- Click on **OK** button to continue or on **Cancel** button to cancel the options.

Output Screen for Sample Sizes for Single-Sample WMW Test (Default Options)

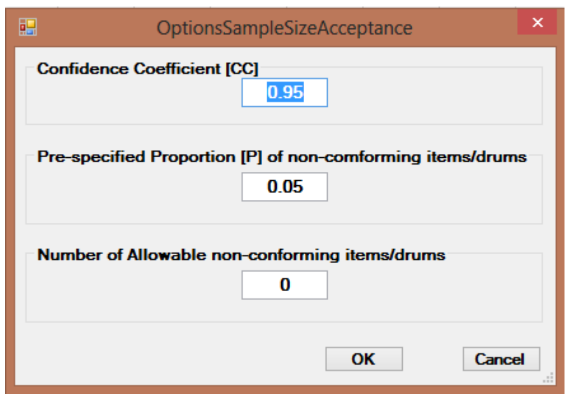
	Sample Sizes for Two Sample Wilcoxon-Mann-Whitney Test
	Based on Specified Values of Decision Parameters/DQOs (Data Quality Objectives)
Date/Time of Computation	2/26/2010 12:18:47 PM
User Selected Options	
False Rejection Rate [Alpha]	0.05
False Acceptance Rate [Beta]	0.1
Width of Gray Region [Delta]	2
Estimate of Standard Deviation	3
	Approximate Minimum Sample Size
Single Sided Alternative Hypothesis:	46
Two Sided Alternative Hypothesis:	56

12.4 Sample Sizes for Acceptance Sampling

1. Click **DQOs Based Sample Sizes ► Acceptance Sampling**



2. The following options window is shown.



- Specify the **Confidence Coefficient.** Default is **0.95**.
- Specify the **Proportion [P] of non-conforming items/drums**. Default is **0.05**.
- Specify the **Number of Allowable non-conforming items/drums**. Default is **0.**
- Click on **OK** button to continue or on **Cancel** button to cancel the options.

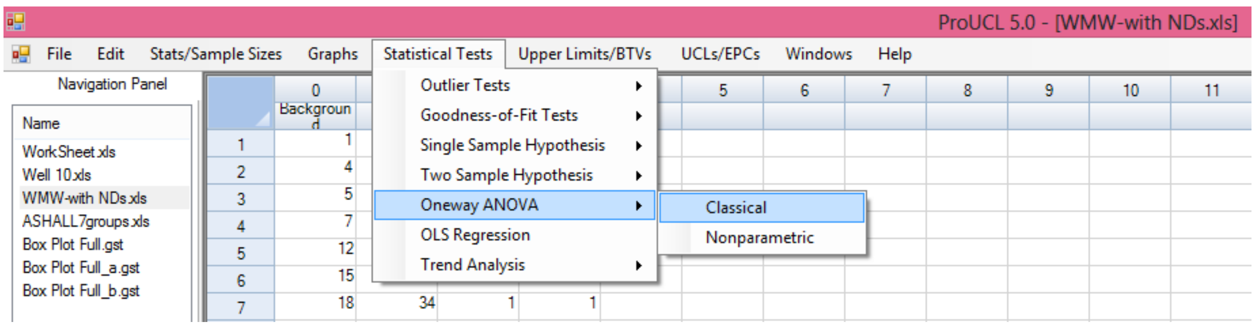
Output Screen for Sample Sizes for Acceptance Sampling (Default Options)

	Acceptance Sampling for Pre-specified Proportion of Non-conforming Items
	Based on Specified Values of Decision Parameters/DQOs
Date/Time of Computation	2/26/2010 12:20:34 PM
User Selected Options	
Confidence Coefficient	0.95
Pre-specified proportion of non-conforming items in the lot	0.05
Number of allowable non-conforming items in the lot	0
	Approximate Minimum Sample Size
Exact Binomial/Beta Distribution	59
Approximate Chisquare Distribution (Tukey-Scheffe)	59

Chapter 13

Analysis of Variance

Oneway Analysis of Variance (ANOVA) is a statistical technique that is used to compare the measures of central tendencies: means or medians of more than two populations/groups. Oneway ANOVA is often used to perform inter-well comparisons in groundwater monitoring projects. Classical Oneway ANOVA is a generalization of the two-sample t-test (Hogg and Craig 1995); and nonparametric ANOVA, Kruskal-Wallis test (Hollander and Wolfe 1999) is a generalization of the two- sample Wilcoxon Mann Whitney test. Theoretical details of Oneway ANOVA are given in the ProUCL Technical Guide. **Oneway ANOVA** is available under the **Statistical Tests** module of ProUCL 5.0/ProUCL 5.1. It is advised to use these tests on raw data in the original scale without transforming the data (e.g., using a log-transformation).



13.1 Classical Oneway ANOVA

1. Click **Oneway ANOVA ► Classical**

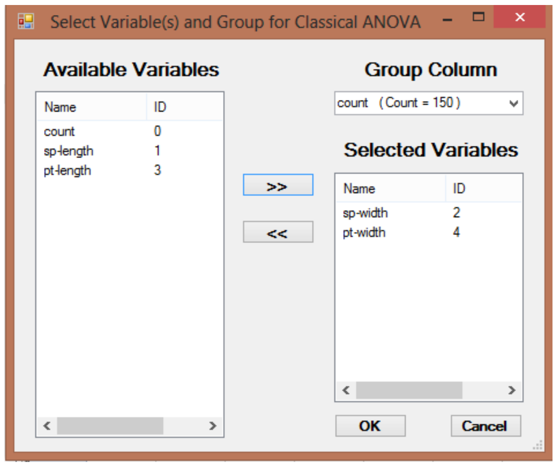
The data file used should follow the format as shown below; the data file should consist of a group variable defining the various groups (stacked data) to be evaluated using the **Oneway ANOVA** module. The **Oneway ANOVA** module can process multiple variables simultaneously.

Well ID	Mn	As
1	460	3
1	527	5
1	579	6
1	541	1
1	518	3.5
8	1350	50
8	1770	61
8	2050	82
8	2420	91
8	1630	31
8	2810	100
9	2200	67
9	2340	82
9	2340	85
9	2420	97
9	2150	130
9	2220	189

2. The **Select Variables** screen will appear.

- Select the variables for testing.
- Select a **Group** variable by using the arrow under the **Group Column** option.
- Click **OK** to continue or **Cancel** to cancel the test.

Example 13-1a. Consider Fisher's (1936) 3 species (groups) Iris flower data set. Fisher collected data on sepal length, sepal width, petal length and petal width for each of the 3 species. Oneway ANOVA results with conclusions for the variable sepal-width (sp-width) are shown as follows:



Output for a Classical Oneway ANOVA

	Classical Oneway ANOVA
Date/Time of Computation	3/26/2013 10:45:03 AM
From File	FULLIRIS-nds.xls
Full Precision	OFF

sp-width

Group	Obs	Mean	SD	Variance
1	50	3.428	0.379	0.144
2	50	2.77	0.314	0.0985
3	50	2.974	0.322	0.104
Grand Statistics (All data)	150	3.057	0.436	0.19

Classical One-Way Analysis of Variance Table

Source	SS	DOF	MS	V.R.(F Stat)	P-Value
Between Groups	11.34	2	5.672	49.16	0
Within Groups	16.96	147	0.115		
Total	28.31	149			

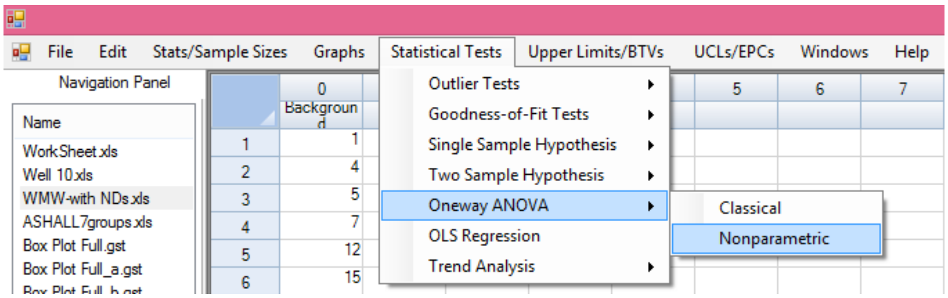
Pooled Standard Deviation	0.34
R-Sq	0.401

Note: A p-value <= 0.05 (or some other selected level) suggests that there are significant differences in mean/median characteristics of the various groups at 0.05 or other selected level of significance
A p-value > 0.05 (or other selected level) suggests that mean/median characteristics of the various groups are comparable.

13.2 Nonparametric ANOVA

Nonparametric Oneway ANOVA or the Kruskal–Wallis (K-W) test is a generalization of the Mann-Whitney two-sample test. This is a nonparametric test and can be used when data from the various groups are not normally distributed.

1. Click Oneway **ANOVA ► Nonparametric**



Like classical Oneway ANOVA, nonparametric ANOVA also requires that the data file used should follow the data format as shown above; the data file should consist of a group variable defining the various groups to be evaluated using the **Oneway ANOVA** module.

2. The **Select Variables** screen will appear.

- Select the variables for testing.
- Select the **Group** variable.
- Click **OK** to continue or **Cancel** to cancel the test.

Example 13-1b (continued). Nonparametric Oneway ANOVA results with conclusion for sepal-length (sp-length) are shown as follows.

Output for a Nonparametric ANOVA

	Nonparametric Oneway ANOVA (Kruskal-Wallis Test)
Date/Time of Computation	3/26/2013 11:11:32 AM
From File	FULLIRIS-nds.xls
Full Precision	OFF

sp-length

Group	Obs	Median	Ave Rank	Z
1	50	5	29.64	-9.142
2	50	5.9	82.65	1.425
3	50	6.5	114.2	7.716
Overall	150	5.8	75.5	

K-W (H-Stat)	DOF	P-Value	(Approx. Chisquare)
96.76	2	0	
96.94	2	0	(Adjusted for Ties)

Note: A p-value <= 0.05 (or some other selected level) suggests that there are significant differences in mean/median characteristics of the various groups at 0.05 or other selected level of significance

A p-value > 0.05 (or other selected level) suggests that mean/median characteristics of the various groups are comparable.

Chapter 14

Ordinary Least Squares of Regression and Trend Analysis

The OLS of regression and trend tests are often used to determine trends potentially present in constituent concentrations at polluted sites, especially in GW monitoring applications. The OLS regression and two nonparametric trend tests: Mann-Kendall test and Theil-Sen test are available under the **Statistical Tests** module of ProUCL 5.0/ProUCL 5.1. The details of these tests can be found in Hollander and Wolfe (1999) and Draper and Smith (1998). Some time series plots, which are useful in comparing trends in analyte concentrations of multiple groups (e.g., monitoring wells), are also available in ProUCL.

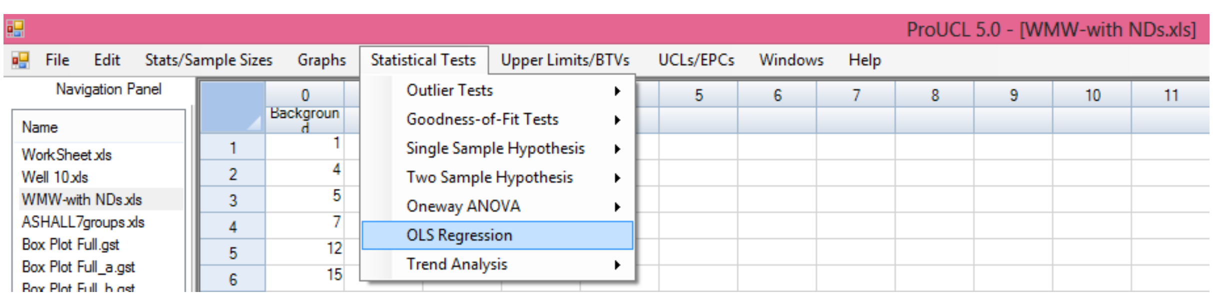
The two nonparametric trend tests: M-K test and Theil-Sen test are meant to identify trends in time series data (data collected over a certain period of time such as daily, monthly, quarterly, etc.) with distinct values of the time variable (time of sampling events). If multiple observations are collected/reported at a sampling event (time), one or more pairwise slopes used in the computation of the Theil-Sen test may not be computed (become infinite). Therefore, it is suggested that the Theil-Sen test only be used on data sets with one measurement collected at each sampling event. If multiple measurements are collected at a sampling event, the user may want to use the average (or median, mode, minimum or maximum) of those measurements resulting in a time series with one measurement per sampling time event. Theil-Sen test in ProUCL has an option which can be used to average multiple observations reported for the various sampling events. The use of this option also computes M-K test statistic and OLS statistics based upon averages of multiple observations collected at the various sampling events.

<u>New in ProUCL 5.1:</u> In addition to slope and intercept of the nonparametric Theil-Sen (T-S) trend line, ProUCL 5.1 computes residuals based upon the T-S trend line.

The trend tests in ProUCL software also assume that the user has entered data in chronological order. If the data are not entered properly in chronological order, the graphical trend displays may be meaningless. **Trend Analysis** and **OLS Regression** modules handle missing values in both response variable (e.g., analyte concentrations) as well as the sampling event variable (called independent variable in OLS).

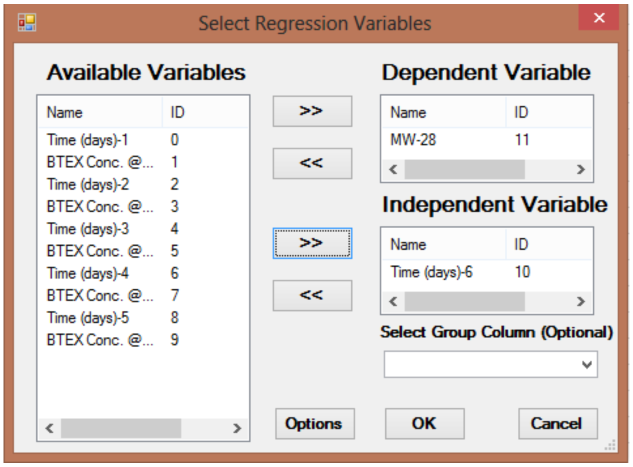
14.1 Simple Linear Regression

1. Click **Statistical Tests► OLS Regression.**



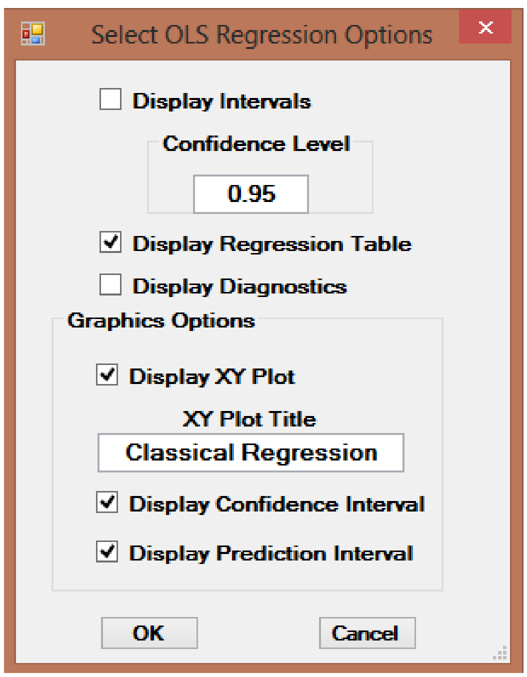
2. The **Select Regression Variables** screen will appear.

- Select the **Dependent Variable** and the **Independent Variable** for the regression analysis.



- Select a group variable (if any) by using the arrow below the **Select Group Column (Optional)**. The analysis will be performed separately for each group.

- When the **Options** button is clicked, the following options window will appear.



  - Select **Display Intervals** for the confidence limits and the prediction limits of each observation to be displayed at the specified **Confidence Coefficient**. The interval estimates will be displayed in the output sheet.

- Select **Display Regression Table** to display Y-hat, residuals and the standardized residuals in the output sheet.

- Select "**XY Plot**" to generate a scatter plot display showing the regression line.

- Select **Confidence Interval** and **Prediction Interval** to display the confidence and the prediction bands around the regression line.

- Click on **OK** button to continue or on **Cancel** button to cancel the option.

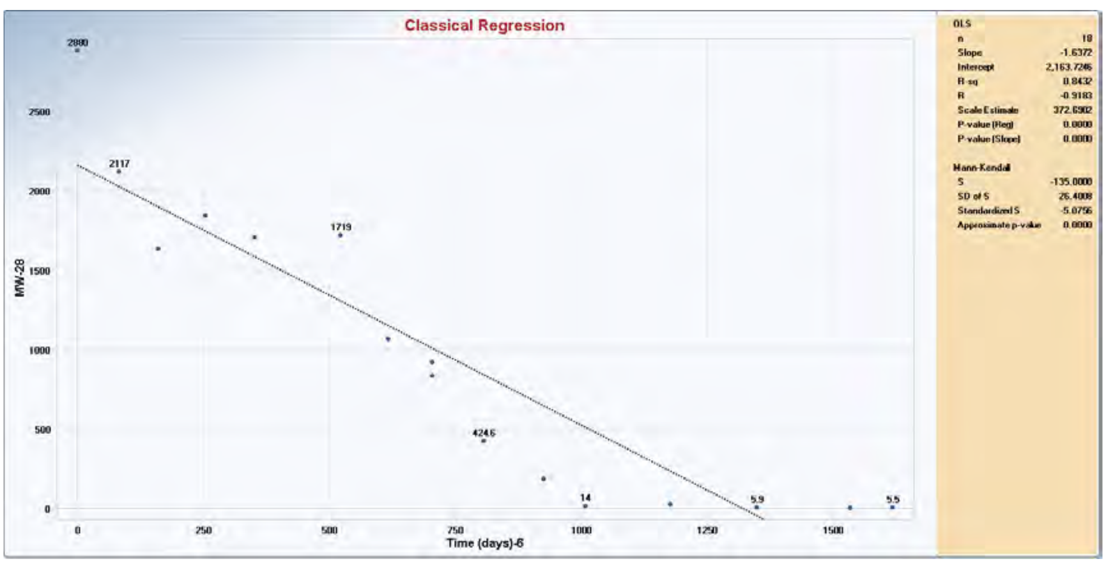
• Click **OK** to continue or **Cancel** to cancel the OLS Regression.

- The use of the above options will display the following graph on your computer screen which can be copied using the **Copy Chart (To Clipboard)** in a Microsoft documents (e.g., word document) using the **File ►Paste** combination.

- The above options will also generate an Excel-Type output sheet. A partial output sheet is shown below following the OLS Regression Graph.

Example 14-1a. Consider analyte concentrations, X collected from a groundwater (GW) monitoring well, MW-28 over a certain period of time. The objective is to determine if there is any trend in GW concentrations, X of the MW-28. The OLS regression line with inference about slope and intercept are shown in the following figure. The slope and its associated *p*-value suggest that there is a significant downward trend in GW concentrations of MW-28.

OLS Regression Graph without Regression and Prediction Intervals



OLS Regression Graph with Regression and Prediction Intervals

Partial Output of OLS Regression Analysis

	Ordinary Least Squares Linear Regression Output Sheet
User Selected Options	
Date/Time of Computation	3/27/2013 11:51:45 AM
From File	Trend-MW-data-use.xls
Full Precision	OFF

Number Reported (x-values)	18
Dependendant Variable	MW-28
Independent Variable	Time (days)-6

Regression Estimates and Inference Table

Paramater	Estimates	Std. Error	T-values	p-values
intercept	2164	165.3	13.09	5.793E-10
ime (days)-6	-1.637	0.176	-9.276	7.7292E-8

OLS ANOVA Table

Source of Variation	SS	DOF	MS	F-Value	P-Value
Regression	11952431	1	11952431	86.05	0.0000
Error	2222368	16	138898		
Total	14174799	17			

R Square	0.843
Adjusted R Square	0.833
Sqrt(MSE) = Scale	372.7

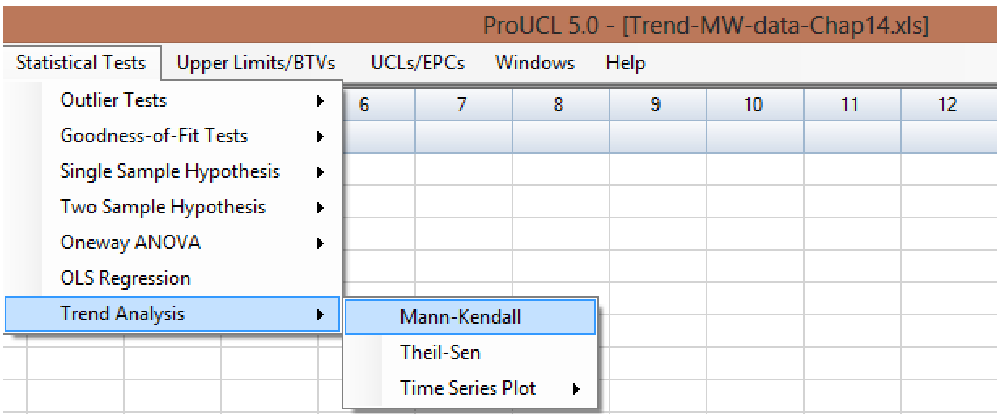
Regression Table

Obs	Y Vector	Yhat	Residuals	Res/Scale
1	2880	2164	716.3	1.922
2	2117	2028	89.17	0.239
3	1633	1900	-267.6	-0.718
4	1845	1748	97.13	0.261
5	1706	1587	118.2	0.317
6	1719	1307	411.1	1.103
7	1065	1154	-88.55	-0.238
8	831.8	1009	-177.7	-0.477
9	920.6	1009	-88.87	-0.238

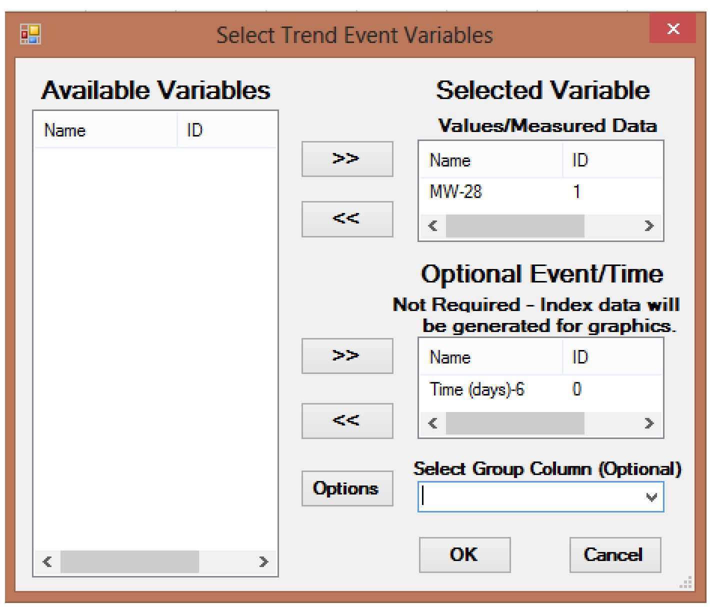
Verifying Normality of Residuals: As shown in the above partial output, ProUCL displays residuals including standardized residuals on the OLS output sheet. Those residuals can be imported (copying and pasting) in an excel file to assess the normality of those OLS residuals. The parametric trend evaluations based upon the OLS slope (significant slope, confidence interval and prediction interval) are valid provided the OLS residuals are normally distributed. Therefore, it is suggested that the user assesses the normality of OLS residuals before drawing trend conclusions using a parametric test based upon the OLS slope estimate. When the assumptions are not met, one can use graphical displays and nonparametric trend tests (e.g., T-S test) to determine potential trends present in a time series data set.

14.2 Mann-Kendall Test

1. Click **Statistical Tests ►Trend Analysis ► Mann-Kendall.**



2. The **Select Trend Event Variables** screen will appear.

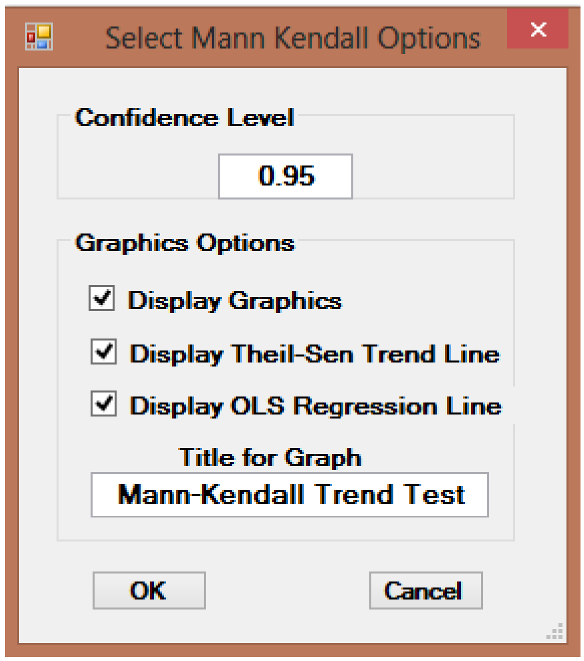


- Select the **Event/Time** variable. This variable is optional to perform the Mann-Kendall (M-K) Test; however, for graphical display it is suggested to provide a valid Event/Time variable (numerical values only). If the user wants to generate a graphical display without providing an Event/Time variable, ProUCL generates an index variable to represent sampling events.

- Select the **Values/Measured Data** variable to perform the trend test.

- Select a group variable (if any) by using the arrow below the **Select Group Column (Optional)**. When a group variable is chosen, the analysis is performed separately for each group represented by the group variable.

- When the **Options** button is clicked, the following window will be shown.



  - Specify the **Confidence Level**; a number in the interval (0.5, 1), 0.5 inclusive. The default choice is **0.95**.

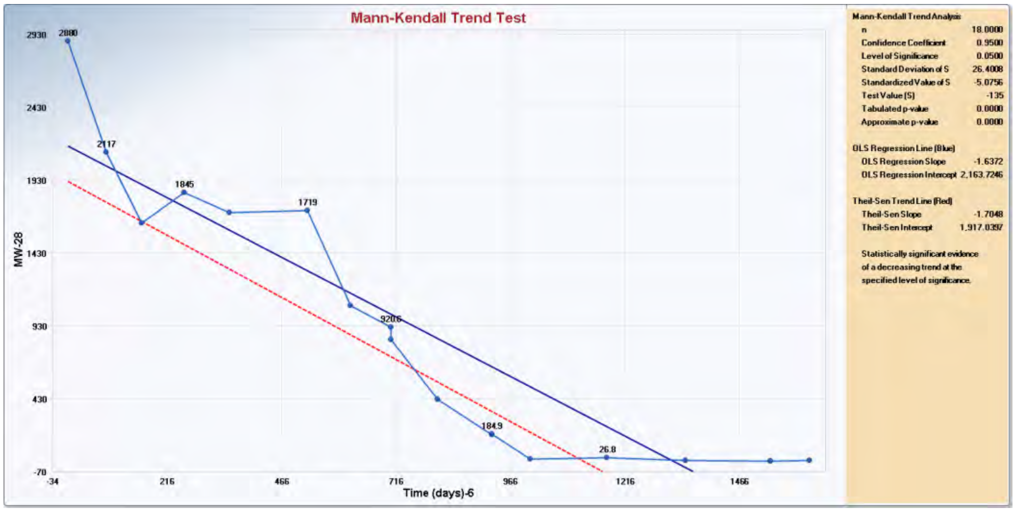
  - Select the trend lines to be displayed: **OLS Regression Line** and/or **Theil-Sen Trend Line**. If only **Display Graphics** is chosen, a time series plot will be generated.

  - Click on **OK** button to continue or on **Cancel** button to cancel the option.

- Click **OK** to continue or **Cancel** to cancel the Mann-Kendall test.

14- 1b (Continued). The M-K test results are shown in the following figure and in the following M-K test output sheet. Based upon the M-K test, it is concluded that there is a statistically significant downward trend in GW concentrations of the MW-28.

Mann Kendall Test Trend Graph displaying all Selected Options



Mann-Kendall Trend Test Output Sheet

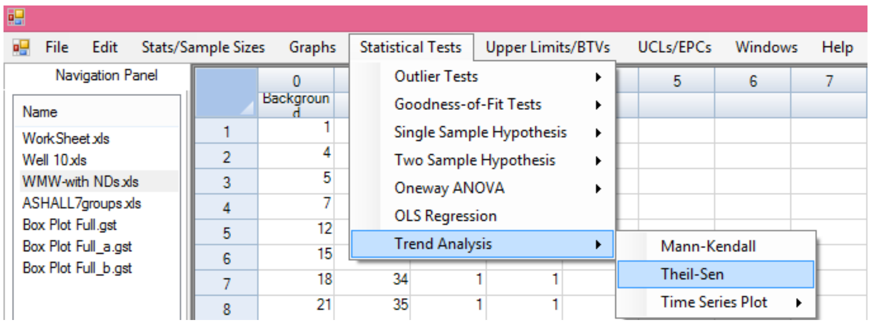
	Mann-Kendall Trend Test Analysis
User Selected Options	
Date/Time of Computation	3/27/2013 12:19:26 PM
From File	Trend-MW-data-Chap14.xls
Full Precision	OFF
Confidence Coefficient	0.95
Level of Significance	0.05

MW-28			
General Statistics			
Number of Events	18		
Number Values Reported (n)	18		
Minimum	1.7		
Maximum	2880		
Mean	864.6		
Geometric Mean	174.8		
Median	628.2		
Standard Deviation	913.1		
Mann-Kendall Test			
Test Value (S)	-135		
Tabulated p-value	0		
Standard Deviation of S	26.4		
Standardized Value of S	-5.076		
Approximate p-value	1.9313E-7		
Statistically significant evidence of a decreasing trend at the specified level of significance.			

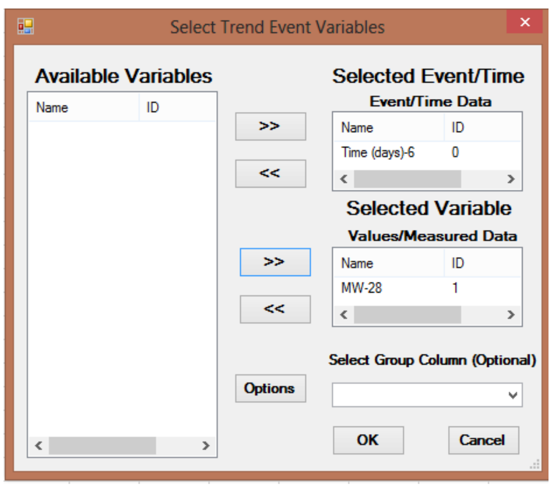
14.3 Theil – Sen Test

To perform the Theil-Sen test, the user is required to provide numerical values for a sampling event variable (numerical values only) as well as values of a characteristic (e.g., analyte concentrations) of interest observed at those sampling events.

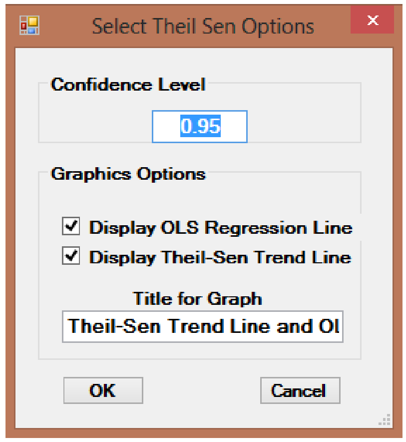
1. Click **Statistical Tests ►Trend Analysis ► Theil-Sen.**



2. The **Select Variables** screen will appear.



- Select an **Event/Time Data** variable.
- Select the **Values/Measured Data** variable to perform the test.
- Select a group variable (if any) by using the arrow below the **Select Group Column (Optional)**. When a group variable is chosen, the analysis is performed separately for each group represented by the group variable.
- When the **Options** button is clicked, the following window will be shown.

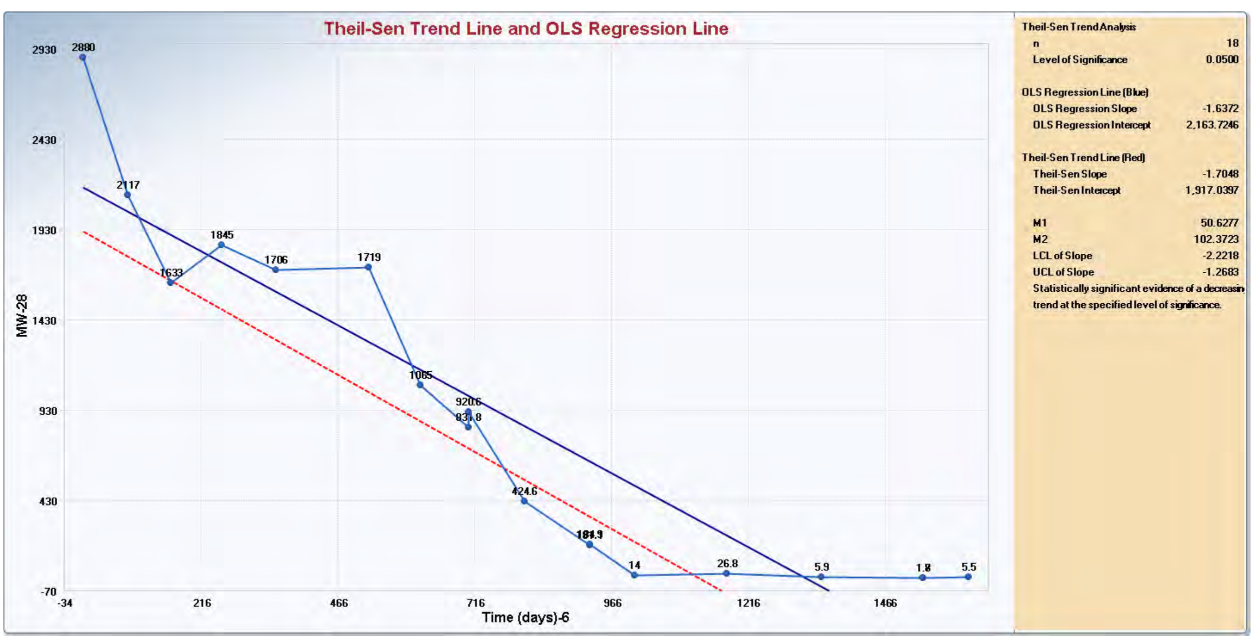


- Specify the **Confidence Level**; a number in the interval (0.5, 1), 0.5 inclusive. The default choice is **0.95**.
- Select the trend lines to be displayed: **OLS Regression Line** and/or **Theil-Sen Trend Line.**
- Click on **OK** button to continue or on **Cancel** button to cancel the option.

- Click **OK** to continue or **Cancel** to cancel the Theil-Sen Test.

14-1c (continued). The Theil-Sen test results are shown in the following figure and in the following Theil-Sen test Output Sheet. It is concluded that there is a statistically significant downward trend in GW concentrations of MW-28. Theil-Sen test results and residuals are summarized in tables following the trend graph shown below.

Theil-Sen Test Trend Graph displaying all Selected Options



Theil-Sen Trend Test Output Sheet

Date/Time of Computation	3/27/2013 2:19:55 PM
From File	Trend-MW-data-Chap14.xls
Full Precision	OFF
Confidence Coefficient	0.95
Level of Significance	0.05

MW-28

General Statistics

Number of Events	18
Number Values Reported (n)	18
Minimum	1.7
Maximum	2880
Mean	864.6
Geometric Mean	174.8
Median	628.2
Standard Deviation	913.1

Approximate inference for Theil-Sen Trend Test

Mann-Kendall Statistic (S)	-137
Standard Deviation of S	26.4
Standardized Value of S	-5.151
Approximate p-value	1.2930E-7
Number of Slopes	153
Theil-Sen Slope	-1.705
Theil-Sen Intercept	1917
M2'	98.21
One-sided 95% upper limit of Slope	-1.365
95% LCL of Slope (0.025)	-2.222
95% UCL of Slope (0.975)	-1.268

Statistically significant evidence of a decreasing trend at the specified level of significance.

Theil-Sen Trend Test Estimates and Residuals

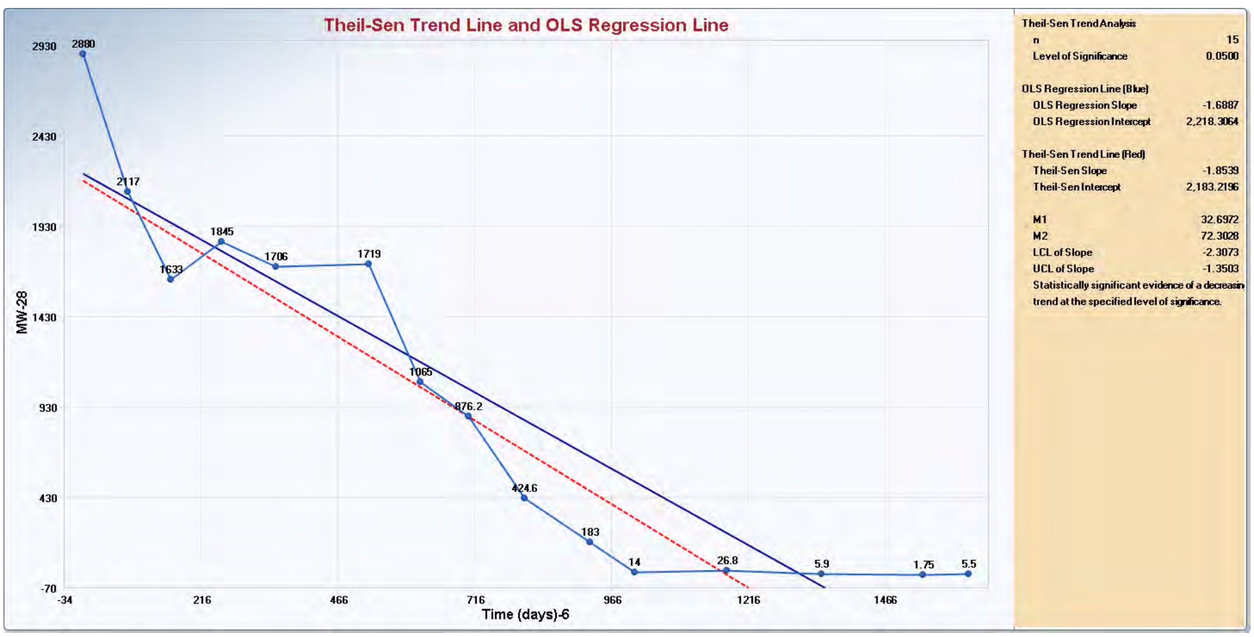
#	Events	Values	Estimates	Residuals
1	0	2880	1917	963
2	83	2117	1776	341.5
3	161	1633	1643	-10.06
4	254	1845	1484	361
5	352	1706	1317	388.7
6	523	1719	1025	693.2
7	617	1065	865.2	199.8
8	705	831.8	715.1	116.7
9	705	920.6	715.1	205.5
10	807	424.6	541.3	-116.7
11	926	181.1	338.4	-157.3
12	926	184.9	338.4	-153.5
13	1009	14	196.9	-182.9
14	1177	26.8	-89.53	116.3
15	1349	5.9	-382.8	388.7
16	1535	1.7	-699.9	701.6
17	1535	1.8	-699.9	701.7
18	1619	5.5	-843.1	848.6

Notes: As with other statistical test statistics, trend test statistics: M-K test statistic, OLS regression and Theil-Sen slopes may lead to different trend conclusions. In such instances it is suggested that the user supplements statistical conclusions with graphical displays.

Averaging of Multiple Measurements at Sampling Events: In practice, when multiple observations are collected/reported at one or more sampling events (times), one or more pairwise slopes may become infinite, resulting in a failure to compute the Theil-Sen test statistic. In such cases, the user may want to pre-process the data before using the Theil-Sen test. Specifically, to assure that only one measurement is available at each sampling event, the user pre-processes the time series data by computing average, median, mode, minimum, or maximum of the multiple observations collected at those sampling events. The Theil-Sen test in ProUCL 5.0/ProUCL 5.1 provides the option of averaging multiple measurements collected at the various sampling events. This option also computes M-K test and OLS regression statistics using the averages of multiple measurements collected at the various sampling event. The OLS regression and M-K test can be performed on data sets with multiple measurements taken at the various sampling time events. However, often it is desirable to use the averages (or median) of measurements taken at the various sampling events to determine potential trends present in a time-series data set.

14-1c (continued). The data set used in Example 14-1c has some sampling events where multiple observations were taken. Theil-Sen test results based upon averages of multiple observations is shown as follows. The data set is included in the ProUCL Data directory which comes with ProUCL 5.1.

Theil-Sen Test Trend Graph displaying all Selected Options
Multiple Observations Taken at Some Sampling Events Have Been Averaged

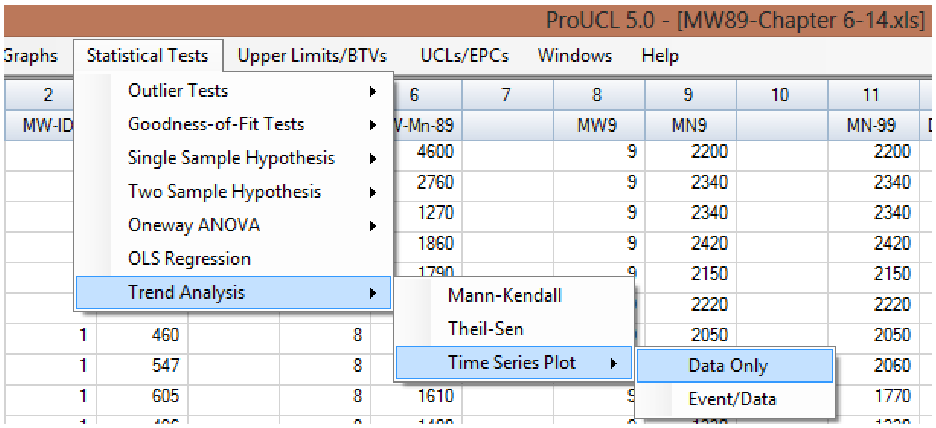


14.4 Time Series Plots

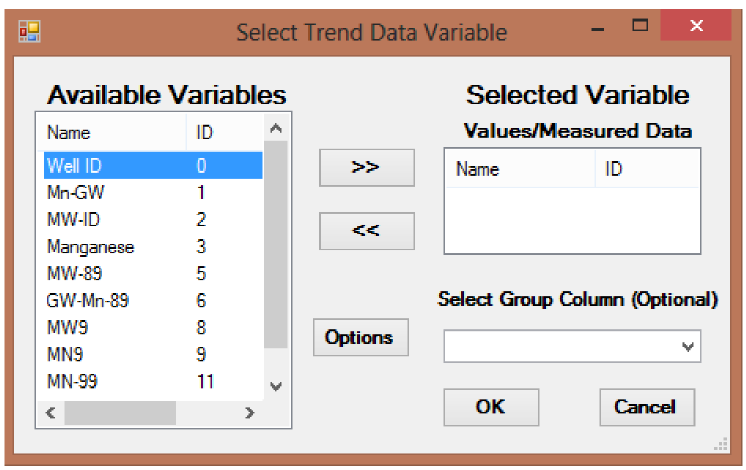
This option of the **Trend Analysis** module can be used to determine and compare trends in multiple groups over the same period of time.

This option is specifically useful when the user wants to compare the concentrations of multiple groups (wells) and the exact sampling event dates are not be available (data only option). The user may just want to graphically compare the time-series data collected from multiple groups/wells during several quarters (every year, every 5 year, etc.). When the user wants to use this module using the **data/event** option, each group (e.g., well) defined by a group variable must have the same number of observations and should share the same sampling event values. That is the number of sampling events and values (e.g., quarter ID, year ID, etc.) for each group (well) must be the same for this option to work. However, the exact sampling dates (not needed to use this option) in the various quarters (years) do not have to be the same as long as the values of the sampling quarters/years (1,3,5,6,7,9,..) used in generating time-series plots for the various groups (wells) match. Using the geological and hydrological information, this kind of comparison may help the project team in identifying non-compliance wells (e.g., with upward trends in constituent concentrations) and associated reasons.

1. Click **Statistical Tests ►Trend Analysis ► Time Series Plots**

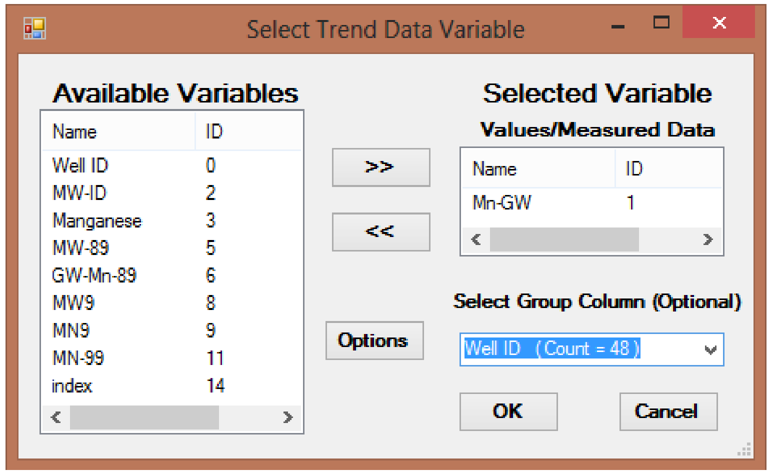


2. When the **Data Only** option is clicked, the following window is shown:

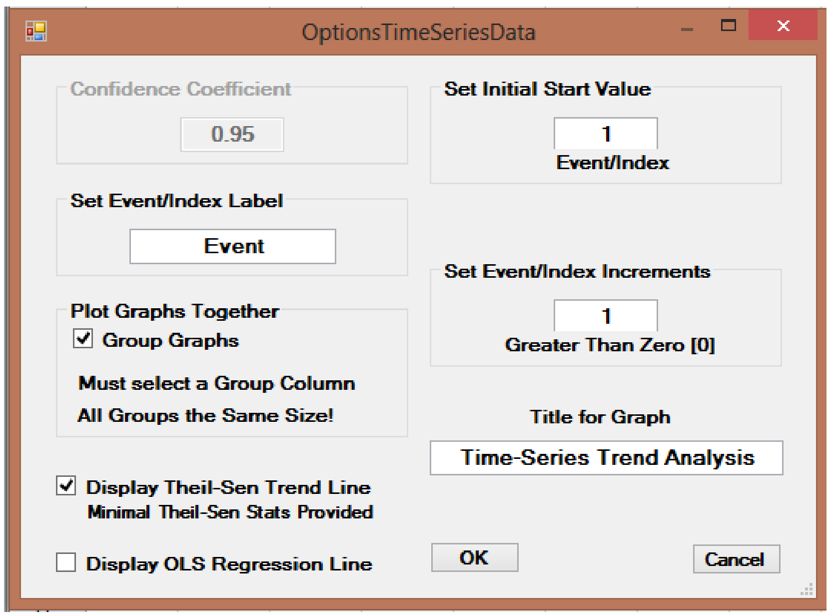


This option is used on the measured data only. The user selects a variable with measured values which are used in generating a time series plot. The time series plot option is specifically useful when data come from multiple groups (monitoring wells during the same period of time).

- Select a group variable (is any) by using the arrow shown below the **Group Column (Optional)**.



- When the **Options** button is clicked, the following window will be shown.



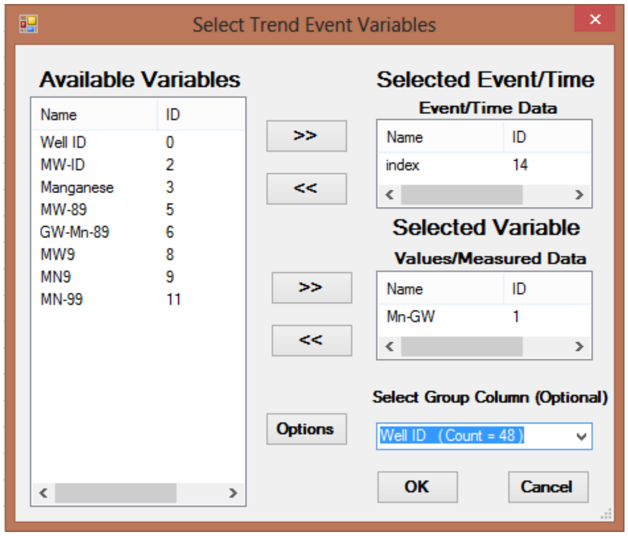
The user can opt to display graphs for each group individually or for all groups together on the same graph by selecting the **Group Graphs** option. The user can also display the OLS line and/or the Theil-Sen line for all groups displayed on the same graph. The user may pick an initial starting value and an increment value to display the measured data. All statistics will be computed using the data displayed on the graphs (e.g., selected **Event** values).

- Input a starting value for the index of the plot using the **Set Initial Start Value**.
- Input the increment steps for the index of the plot using the **Set Index/Event Increments**.
- Specify the lines (**Regression** and/or **Theil-Sen**) to be displayed on the time series plot.
- Select **Plot Graphs Together** option for comparing the time series trends for more than one group on the same graph.

- If this option is not selected but a **Group Variable** is selected, different graphs will be plotted for each group.

- Click on **OK** button to continue or on **Cancel** button to cancel the Time Series Plot.

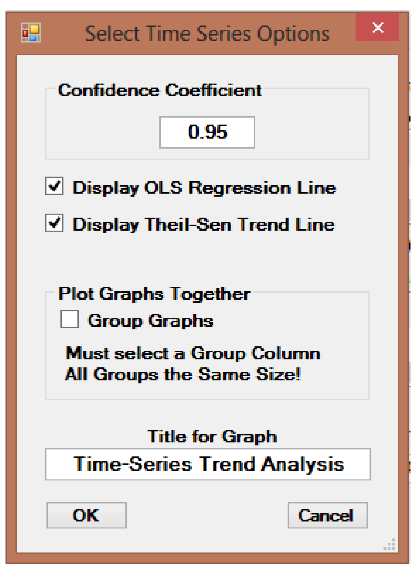
3. When the **Event/Data** option is clicked, the following window is shown:



- Select a group variable (is any) by using the arrow shown below the **Group Column (Optional)**.

- This option uses both the Measured Data and the Event/Time Data. The user selects two variables; one representing the Event/Time variable and the other representing the Measured Data values which will be used in generating a time series plot.

- When the **Options** button is clicked, the following window will be shown.



The user can select to display graphs individually or together for all groups on the same graph by selecting the **Plot Graphs Together** option. The user can also display the OLS line and/or the Theil-Sen line for all groups displayed on the same graph.

- Specify the lines (**Regression** and/or **Theil-Sen**) to be displayed on the time series plot.

- Select **Plot Graphs Together** option for comparing time series trends for more than one group on the same graph.

- If this option is not selected but a **Group Variable** is selected, different graphs will be plotted for each group.

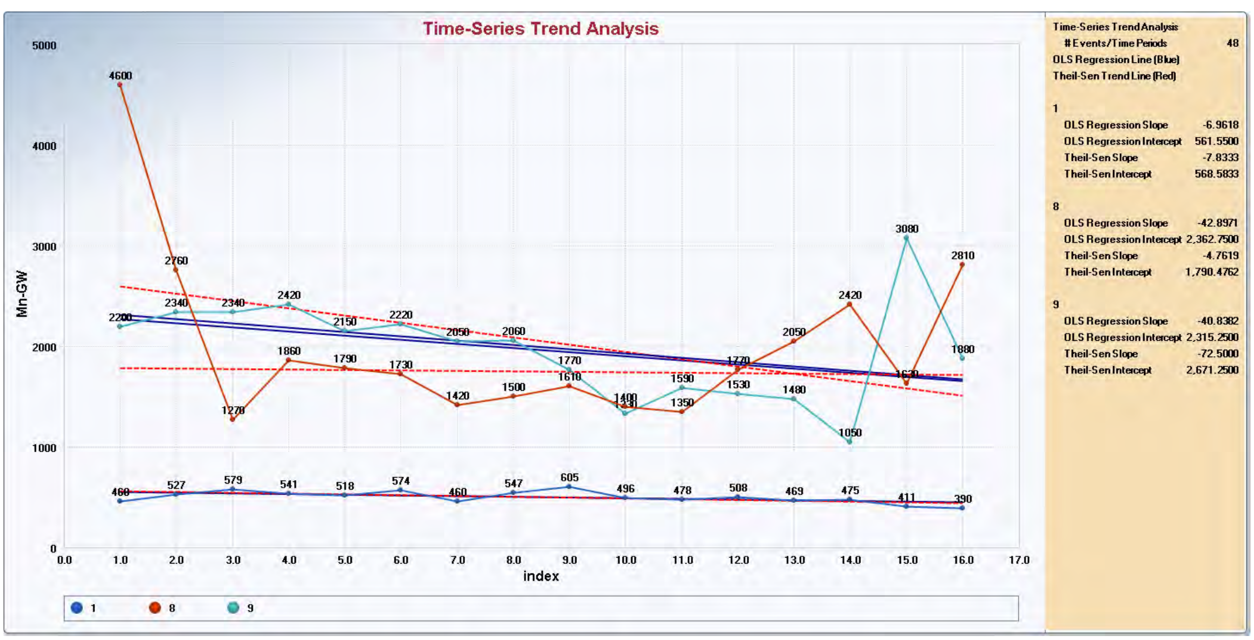
- Click on **OK** button to continue or on **Cancel** button to cancel the options.

- Click **OK** to continue or **Cancel** to cancel the Time Series Plot.

Notes: To use this option, each group (e.g., well) defined by a group variable must have the same number of observations and should share the same sampling event values (if available). That is the sampling events (e.g., quarter ID, year ID, etc.) for each group (well) must be the same for this option to work. Specifically, the exact sampling dates within the various quarters (years) do not have to be the same as long as the sampling quarters (years) for the various wells match.

Example 14-2. The following graph has three (3) time series plots comparing manganese concentrations of the three GW monitoring wells (1 upgradient well [MW1] and 2 downgradient wells [MW8 and MW9]) over the period of 4 years (data collected quarterly). Some trend statistics are displayed in the side panel.

Output for a Time Series Plot – Event/Data Option by a Group Variable (1, 8, and 9)



Chapter 15

Background Incremental Sample Simulator (BISS) Simulating BISS Data from a Large Discrete Background Data

The **Background Incremental Sample Simulator** (**BISS**) module was incorporated in ProUCL5.0 at the request of the Office of Superfund Remediation and Technology Innovation (OSRTI). However, this module is currently under further investigation and research, and therefore it is not available for general public use. This module has been retained in ProUCL 5.1. This module may be released in a future version of the ProUCL software, along with strict conditions and guidance for how it is applied. The main text for this chapter is not included in this document for release to general public. Only a brief placeholder write-up is provided here.

The following scenario describes the Site or project conditions under which the BISS module could be useful: Suppose there is a long history of soil sample collection at a Site. In addition to having a large amount of Site data, a robust background data set (at least 30 samples from verified background locations) has also been collected. Comparison of background data to on-Site data has been, and will continue to be, an important part of this project's decision-making strategy. All historical data is from discrete samples, including the background data. There is now a desire to switch to incremental sampling for the Site. However, guidance for incremental sampling makes it clear that it is inappropriate to compare discrete sample results to incremental sample results. That includes comparing a Site's incremental results directly to discrete background results.

One option is to recollect all background data in the form of incremental samples from background DUs that are designed to match Site DUs in geology, area, depth, target soil particle size, number of increments, increment sample support, etc. If project decision-making uses a BTV strategy to compare Site DU results one at a time against background, then an appropriate number (the default is no less than 10) of background DU incremental samples would need to be collected to determine the BTV for the population of background DUs. However, if the existing discrete background data show background concentrations to be low (in comparison to Site concentrations) and fairly consistent (relative standard deviation, RSD <1), there is a second option described as follows.

When a robust discrete background data set that meets the above conditions already exists, the following is an alternative to automatically recollecting ALL background data as incremental samples.

Step 1. Identify 3 background DUs and collect at least 1 incremental sample from each for a minimum of 3 background incremental samples.

Step 2. Enter the discrete background data set ($n \geq 30$) and the ≥3 background incremental samples into the **BISS** module (the **BISS** module will not run unless both data sets are entered).

- The **BISS** module will generate a specified (default is 7) simulated incremental samples from the discrete data set.

- The module will then run a t-test to compare the simulated background incremental data set (e.g., with $n = 7$) to the actual background incremental data set ($n \geq 3$).

- If the t-test finds no difference between the 2 data sets, the **BISS** module will combine the 2 data sets and determine the statistical distribution, mean, standard deviation, potential UCLs and potential BTVs for the combined data set. Only this information will be supplied to the general user. The individual values of the simulated incremental samples will not be provided.

- If the t-test finds a difference between the actual and simulated data sets, the BISS module will not combine the data sets nor provide a BTV.

- In both cases, the BISS module will report summary statistics for the actual and simulated data sets.

Step 3. If the **BISS** module reported out statistical analyses from the combined data set, select the BTV to use with Site DU incremental sample results. Document the procedure used to generate the BTV in project reports. If the **BISS** module reported that the simulated and actual data sets were different, the historical discrete data set cannot be used to simulate incremental results. Additional background DU incremental samples will need to be collected to obtain a background DU incremental data set with the number of results appropriate for the intended use of the background data set.

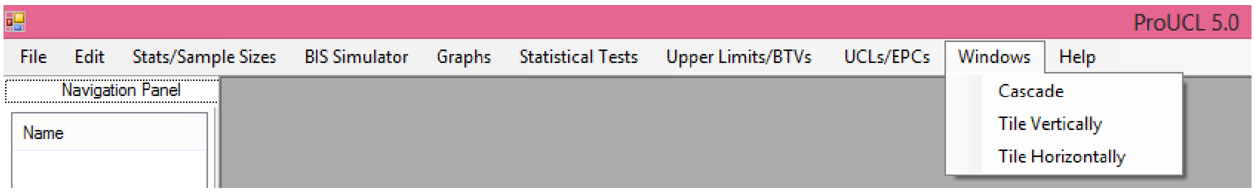
The objective of the **BISS** module is to take advantage of the information provided by the existing background discrete samples. The availability of a large discrete data set collected from the background areas with geological formations and conditions comparable to the Site DU(s) of interest is a requirement for successful application of this module. There are fundamental differences between incremental and discrete samples. For example, the sample supports of discrete and incremental samples are very different. Sample support has a profound effect on sample results so samples with different sample supports should not be compared directly, or compared with great caution.

Since incremental sampling is a relatively new approach, the performance of the **BISS** module requires further investigation. If you would like to try this strategy for your project, or if you have questions, contact Deana Crumbling, crumbling.deana@epa.gov.

Chapter 16

Windows

The Windows Menu performs typical Windows program options.



Click on the **Window** menu to reveal the drop-down options shown above.

The following Window drop-down menu options are available:

- Cascade option: arranges windows in a cascade format. This is similar to a typical Windows program option.

- Tile option: resizes each window vertically or horizontally and then displays all open windows. This is similar to a typical Windows program option.

- The drop-down options list also includes a list of all open windows with a check mark in front of the active window. Click on any of the windows listed to make that window active. This is especially useful if you have many windows (e.g., >40) open; the navigation panel only holds the first 40 windows.

Chapter 17

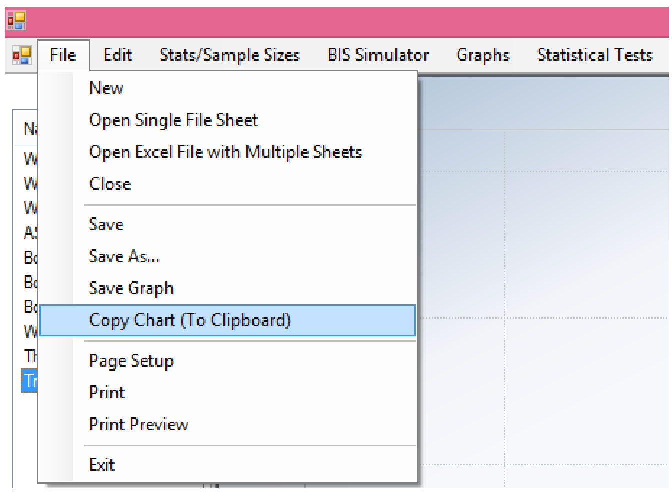
Handling the Output Screens and Graphs

17.1 Copying and Saving Graphs

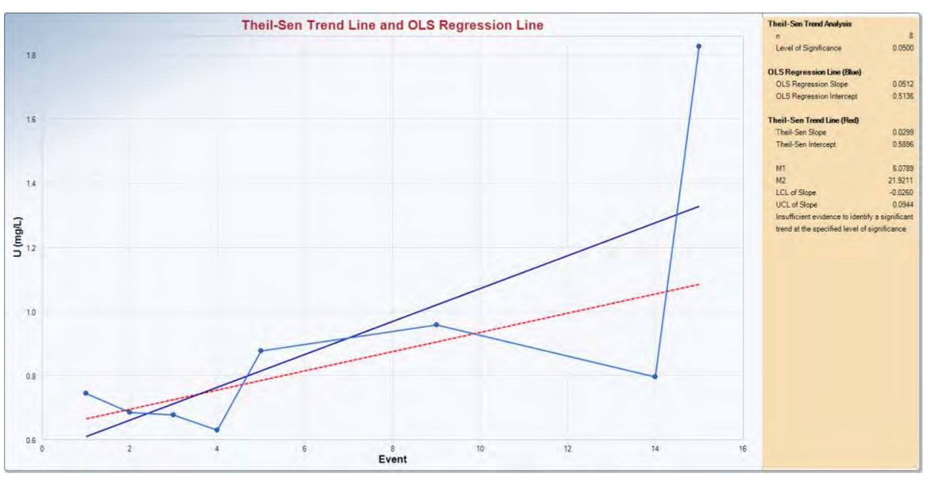
Graphs can be copied into Word, Excel, or PowerPoint files in two ways.

1. Click the **Copy Chart (To Clipboard)** shown below; a graph must be present to be copied to the clipboard.

File ► Copy Chart (To Clipboard)

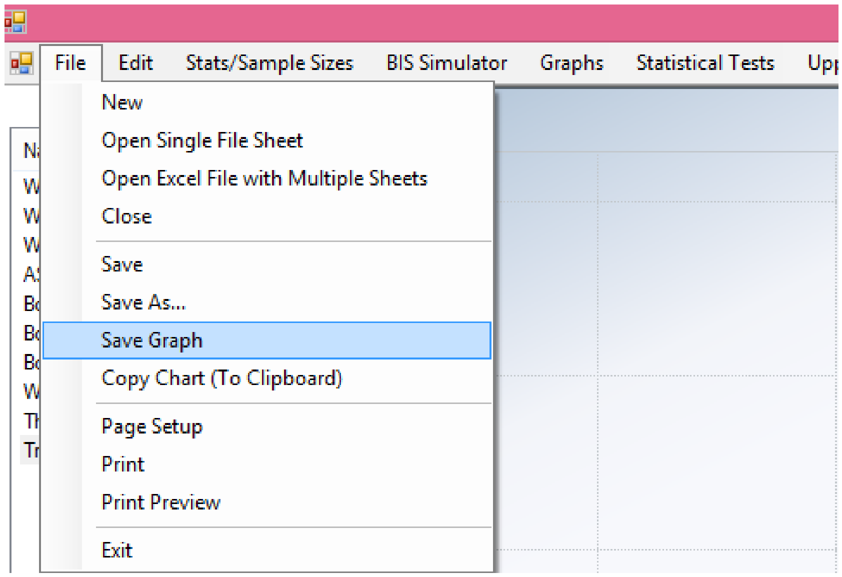


Once the user has clicked **Copy Chart (To Clipboard)**, the graph is ready to be imported (pasted) into most Microsoft office applications (e.g., Word, Excel, and PowerPoint) by clicking the **Edit ► Paste** option in those Microsoft applications as shown below.



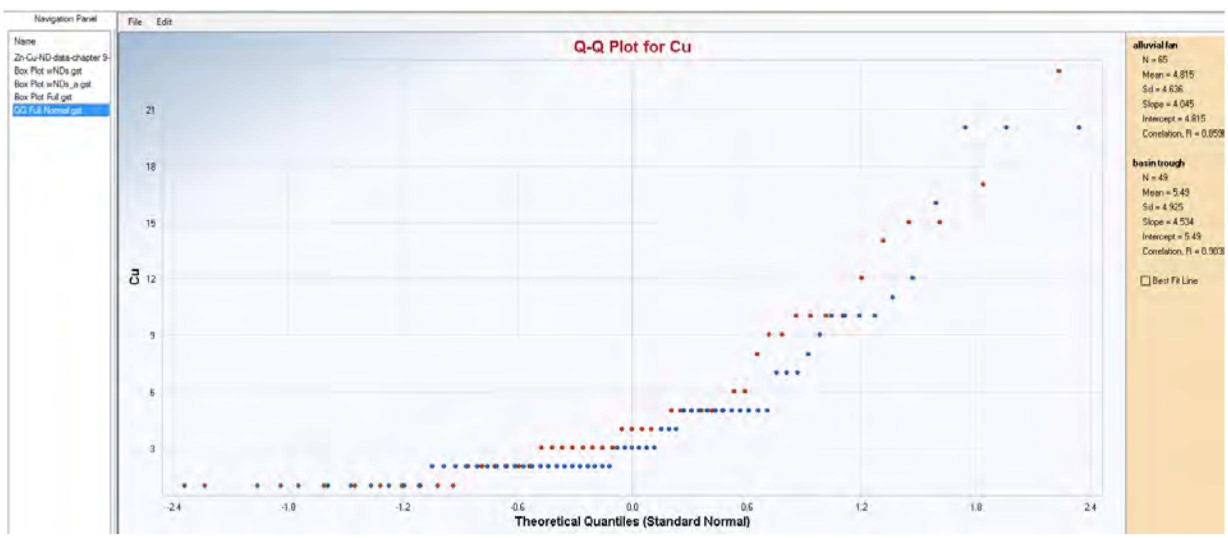
2. Graphs can be saved using the **Save Graph** Option in the **Navigation Panel** as a **Bitmap file** with .bmp extension. The user can import the saved bitmap file into a desired document such as a word document or a PowerPoint presentation by using the **Copy** and **Paste** options available in the selected Microsoft application.

File ► Save Graph

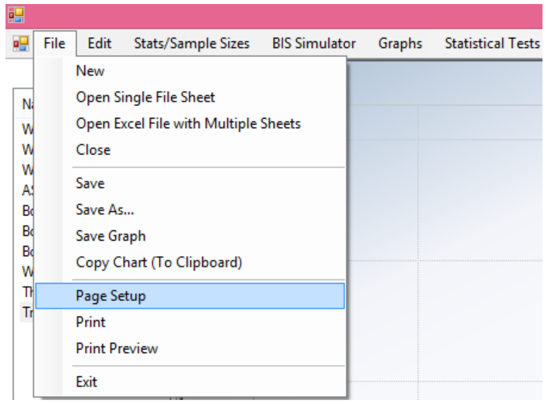


17.2 Printing Graphs

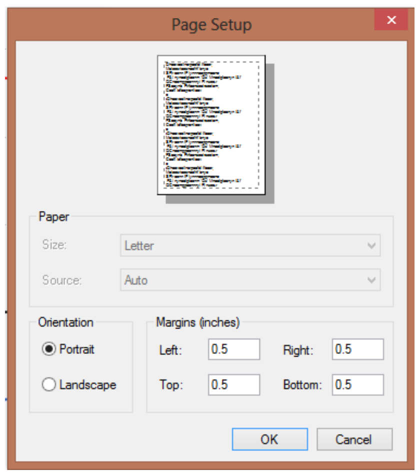
1. Click the graph you want to print in the **Navigation Panel**.



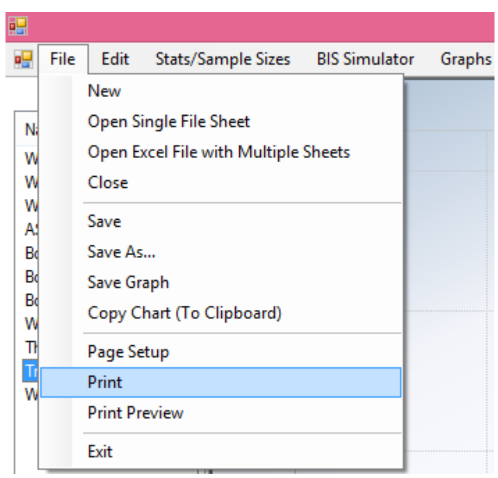
2. Click **File** ▶ **Page Setup**.



3. Check the button next to **Portrait** or **Landscape** (shown below), and click **OK**. In some cases, with larger headings and captions, it may be desirable to use the **Landscape** printing option.



4. Click **File** ▶ **Print** to print the graph, and **File** ▶ **Print Preview** to preview (optional) the graph before printing.



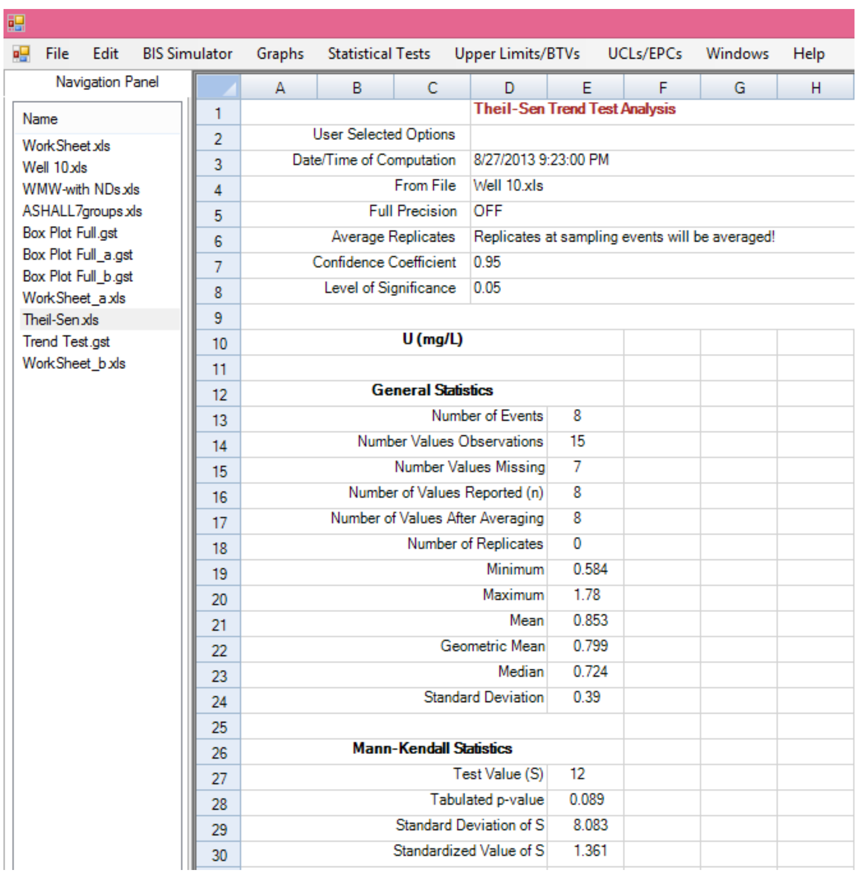
17.3 Making Changes in Graphs using Tools and Properties

ProUCL uses a couple of development tools such as FarPoint spread (for Excel type input and output operations) and ChartFx (for graphical displays). ProUCL generates box plots using the built-in box plot feature in ChartFx. The programmer has no control over computing various statistics (e.g., Q1, Q2, Q3, IQR) using ChartFx. So box plots generated by ProUCL can differ slightly from box plots generated by other programs (e.g., Excel). Box plots generated using ChartFx round values to the nearest integer. For increased precision of graphical displays (all graphical displays generated by ProUCL), the user can use the process described as follows.

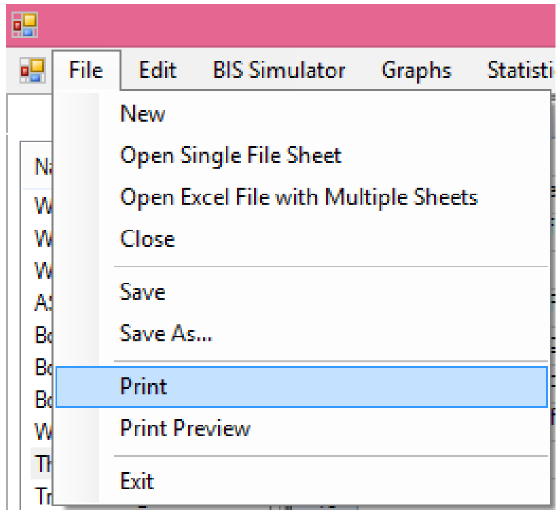
Position your mouse cursor on the graph and right-click, a popup menu will appear. Position the mouse on **Properties** and right-click; a windows form labeled **Properties** will appear. There are three choices at the top; General, Series and Y-Axis. Position the mouse cursor over the Y-Axis choice and left-click. You can change the number of decimals to increase the precision, change the step to increase or decrease the number Y-Axis values displayed and/or change the direction of the label. To show values on the plot itself, position your mouse cursor on the graph and right-click; a popup menu will appear. Position the mouse on Point Labels and right-click. There are other options available in this popup menu including changing font sizes.

17.4 Printing Non-graphical Outputs

1. Click/Highlight the output you want to save or print in the **Navigation Panel**.



2. Click **File ► Print** or **File ► Print Preview** if you wish to see the preview before printing.

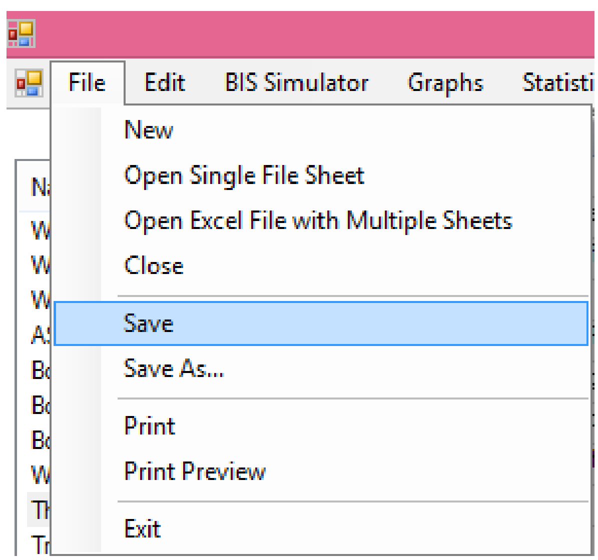


17.5 Saving Output Screens as Excel Files

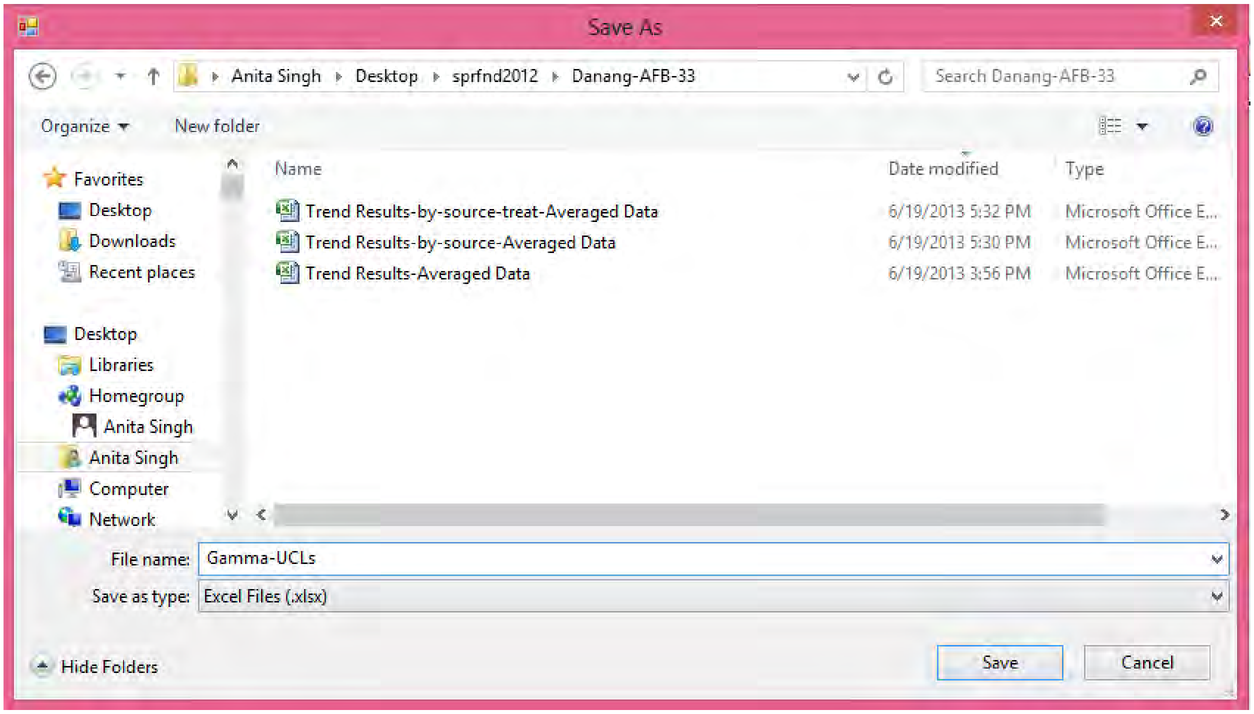
ProUCL 5.0/ProUCL 5.1 saves output files and data files as Excel files with .xls or .xlsx extensions.

1. Click on the output you want to save in the **Navigation Panel List**.

2. Click **File ► Save** or **File► Save As**



3. Enter the desired file name you want to use, and click **Save**, and save the file in the desired folder using your browser as shown below.


Save As
Anita Singh ▸ Desktop ▸ sprfnd2012 ▸ Danang-AFB-33
Search Danang-AFB-33
Organize
New folder
Favorites
Desktop
Downloads
Recent places
Desktop
Libraries
Homegroup
Anita Singh
Anita Singh
Computer
Network
Name
Date modified
Type
Trend Results-by-source-treat-Averaged Data
6/19/2013 5:32 PM
Microsoft Office E...
Trend Results-by-source-Averaged Data
6/19/2013 5:30 PM
Microsoft Office E...
Trend Results-Averaged Data
6/19/2013 3:56 PM
Microsoft Office E...
File name:
Gamma-UCLs
Save as type:
Excel Files (.xlsx)
Hide Folders
Save
Cancel

Chapter 18

Summary and Recommendations to Compute a 95% UCL for Full Uncensored and Left-Censored Data Sets with NDs

This chapter briefly summarizes recommendations and the process to compute upper confidence limits of the population mean based upon data sets with and without ND observations. The recommendations are made based upon the simulation studies summarized in Singh, Singh, and Engelhardt (1997, 1999); Singh, Singh, and Iaci (2002); Singh and Singh (2003); and Singh, Maichle, and Lee (2006). Some details can be found in Chapters 2 and 4 of the associated ProUCL 5.1 Technical Guide. Depending upon the data size, data distribution (e.g., normal, gamma, lognormal, and nonparametric), and data skewness, ProUCL suggests using one or more 95% UCL to estimate the population mean. The project team collectively should determine which of the suggested UCLs will be most appropriate for their project. If needed, the user may want to consult a statistician for additional insight.

18.1 Computing UCL95s of the Mean Based Upon Uncensored Full Data Sets

- Formal GOF tests and GOF Q-Q plots are used first to determine the data distribution so that appropriate parametric or nonparametric UCL95s can be computed.

- For a normally or approximately normally distributed data set, the user is advised to use Student's t-distribution-based UCL of the mean. Student's t UCL or modified-t-statistic based UCL can be used to estimate the EPC when the data set is symmetric (e.g., skewness = $\left|\hat{k}_3\right|$ is smaller than 0.2-0.3) or mildly skewed; that is, when σ or $\hat{\sigma}$ is less than 0.5. In practice, for mildly skewed data sets (with *sd* of logged data <0.5), all parametric UCLs computation methods available in ProUCL tend to yield comparable results.

- For gamma or approximately gamma distributed data sets, the user is advised to: 1) use the approximate gamma UCL when k>1 and $n \geq 50$; 2) use the adjusted gamma UCL when $k>1$ and $n<50$; 3) use the bootstrap-t method or Hall's bootstrap method when $k \leq 1$ and the sample size, $n < 15\text{-}20$; 4) use approximate gamma UCL for $k \leq 1$ and sample size, $n \geq 50$; and 5) use the adjusted gamma UCL (if available) for $k \leq 1$ and sample size, $50 > n \geq 15$. If the adjusted gamma UCL is not available (e.g., when an unusual CC level such as 0.935 is selected), then use the approximate gamma UCL as an estimate of the EPC. When the bootstrap-t method or Hall's bootstrap method yields an erratic inflated UCL (e.g., when outliers are present) result, the UCL may be computed using the adjusted gamma UCL (if available) or the approximate gamma UCL.

- For lognormally distributed data sets, ProUCL recommends a UCL computation method based upon the sample size, n, and standard deviation of the log-transformed data, $\hat{\sigma}$. These suggestions are summarized in Table 2-10 of the ProUCL 5.1 Technical Guide.

- For nonparametric data sets, which are not normally, lognormally, or gamma distributed, a nonparametric UCL is used to estimate the EPC. Methods used to estimate EPC terms based upon nonparametric data sets are summarized in Table 2-11 of the ProUCL 5.1 Technical Guide. For example for mildly skewed nonparametric data sets of smaller sizes (e.g., <30), one may use a modified-t UCL or BCA bootstrap UCL; and for larger samples one may use a CLT-UCL, adjusted-CLT UCL, or a BCA bootstrap UCL. These nonparametric UCLs computation methods do not provide desired coverage to the mean for moderately skewed to highly skewed data sets.

- For moderately skewed to highly skewed nonparametric data sets, the use of a Chebyshev (Mean, *Sd*) UCL is suggested. It is noted that for extremely skewed data sets (e.g., with $\hat{\sigma}$ exceeding 3.0), even a Chebyshev inequality-based 99% UCL of the mean fails to provide the desired coverage (e.g., 0.95) of the population mean.

- For highly skewed data sets with $\hat{\sigma}$ exceeding 3.0, 3.5, pre-processing the data is suggested. It is very likely that the data consist of outliers and/or come from multiple populations. The population partitioning methods may be used to identify mixture populations present in the data set. For defensible conclusions, the decision statistics such as EPC terms may be computed separately for each of the identified sub-population present in the mixture data set.

18.2 Computing UCLs Based Upon Left-Censored Data Sets with Nondetects

The parametric maximum likelihood estimation (MLE) methods (e.g., Cohen 1991) and expectation maximization (EM) method (Gleit 1985) assume normality or lognormality of data sets and tend to work only when the data set has NDs with only one detection limit. These days, due to modern analytical tools and equipment, an environmental data sets consists of NDs with multiple detection limits. Since it is not easy to verify (perform goodness-of-fit) the distribution of a left-censored data set consisting of detects and NDs with multiple detection limits, some poor performing estimation methods including the parametric MLE and EM methods and the winsorization method are not retained in ProUCL 5.0/ProUCL 5.1. In ProUCL, emphasis is given to the use of nonparametric UCL computation methods and hybrid parametric methods based upon KM estimates which account for data skewness in the computation of UCL95. Avoid the use of transformations (to achieve symmetry) while computing upper limits based upon left-censored data sets. It is not easy to correctly interpret the statistics computed in the transformed scale. Moreover, the results and statistics computed in the original scale do not suffer from transformation bias. Like full uncensored data sets, when the standard deviation of the log-transformed data becomes >1.0, avoid the use of a lognormal model even when the data appear to be lognormally distributed. Its use often results in unrealistic statistics of no practical merit (Singh, Singh, and Engelhard 1997; Singh, Singh, and Iaci 2002). It is also recommended to identify potential outliers representing observations coming from population(s) different from the main dominant population and investigate them separately. Decisions about the disposition of outliers should be made by all interested members of the project team.

- It is recommended to avoid the use of the DL/2 (t) UCL method, as the DL/2 UCL does not provide the desired coverage (for any distribution and sample size) for the population mean, even for censoring levels as low as 10%, 15%. This is contrary to the conjecture and assertion (e.g., EPA 2006a) made that the DL/2 method can be used for lower (e.g., ≤ 20%) censoring levels. The coverage provided by the DL/2 (t) method deteriorates fast as the censoring intensity increases. The DL/2 (t) method is not recommended by the authors or developers of this text and ProUCL software.

- The use of the KM estimation method is a preferred method as it can handle multiple detection limits. Therefore, the use of KM estimates is suggested to compute the decision statistics based upon methods which adjust for data skewness. Depending upon the data set size, distribution of the detected data, and data skewness, the various nonparametric and hybrid KM UCL95 methods including KM (BCA), bootstrap-t KM UCL, Chebyshev KM

UCL, Gamma-KM UCL based upon the KM estimates provide good coverages for the population mean. All of these methods are available in ProUCL 5.1.

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